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The model, which consists of seven computational modules, simulates the environmental concentrations of pesticides in air, ephemeral surface ponds, soil, soil water and soil gas, plant roots and aboveground plant biomass, and animals in the food chain. These media serve as vectors for end-point species exposure to pesticides. The model computes both toxicant loadings to, and whole body concentrations in, the end-point species. To compute the probability of wildlife exposures to these environmental concentrations, the model is equipped with a Monte Carlo pre- and post-processing capability. The model documentation contains a discussion of model theory, code installation and execution, parameter guidance and programmer's-level model description. Also described is ATTEAM, a symplified analytical version of the food chain portions of the model.

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TERRESTRIAL ECOSYSTEM
EXPOSURE ASSESSMENT MODEL (TEEAM)

by

J.D. Dean, K.A. Voos, R.W. Schanz, and B.P. Popenuck

Woodward-Clyde Consultants
500 12th Street, Suite 100
Oakland, CA 94607-4014

Contract No. 68-03-6304

Project Officer
Lee A. Mulkey
Assessment Branch
Environmental Research Laboratory
Athens, GA 30613-7799

ENVIRONMENTAL RESEARCH LABORATORY
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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient analytical tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Assessment Branch develops management or engineering tools for exposure and risk evaluations of pesticides and other toxic substances.

In this work, a simulation model for toxic chemical exposures to terrestrial wildlife was developed as part of the Ecological Risk Assessment Research Program. The initial focus of the Terrestrial Ecosystem Exposure Assessment Model was on pesticide threats to small- and medium-sized birds in agricultural settings. Using TEEAM, the environmental analyst can compute the probability of wildlife exposure in evaluating the registration or regulation of specific pesticides.

Rosemarie C. Russo, Ph.D.
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

The Terrestrial Ecosystem Exposure Assessment Model is a computer code that simulates toxic organic chemical exposures to wildlife. The approach was to build a code generally applicable to a diverse range of terrestrial ecosystems that could be parameterized to represent various ecosystem types. The initial focus, however, was on pesticide exposure to small and medium-size birds in agricultural settings. Using TEEAM, the environmental analyst can compute the probability of wildlife exposure in evaluating the registration or regulation of pesticides.

The model, which consists of seven computational modules, simulates the environmental concentrations of pesticides in air, ephemeral surface ponds, soil, soil water and soil gas, plant roots and aboveground plant biomass, and animals in the terrestrial food chain. These media serve as vectors for end-point species exposure to pesticides. The model computes both toxicant loadings to, and whole body concentrations in, the end-point species. To compute the probability of wildlife exposures to these environmental concentrations, the model is equipped with a Monte Carlo pre- and post-processing capability.

The model documentation contains a discussion of model theory, code installation and execution, parameter guidance and programmer's-level model description. Also described is ATEEAM, a simplified analytical version of the food chain portions of the model.

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CONTENTS

Page

Disclaimer. ii
Foreword iii
Tables ix
Figures xii
Acknowledgments xiv

Section

1.0 Introduction 1

1.1 Background 1
1.2 Objectives and Scope 1
1.2.1 Long-Term Ecological Changes 2
1.2.2 Short-Term Toxicant-Induced Ecusystem Changes . . . 2
1.2.3 Typical MOdel Applications 4
1.2.4 Priority Ecosystems 5
1.2.5 Outputs of Interest 5
1.2.6 Chemical Release Scenarios 6
1.3 Report Organization 6

2.0 Model Overview 7

2.1 Previous Work 7
2.2 Model Features 9
2.2.1 Proceses Simulated 9
2.2.2 Model Spatial Features 13
2.2.3 Model Temporal Features 15
2.2.4 Software Features 17
2.3 Recommendations for Further Work 18
2.3.1 Additions to Existing Code 18
2.3.2 Parameter Estimation and Model Verification 19

3.0 TEEAM Modules and Processes 20

3.1 Toxicant Application/Deposition Submodel 20
3.1.1 Introduction 20
3.1.2 Module Development 25
3.2 Terrestrial Fate and Transport Module (TFAT) 40
3.2.1 The Basic Fate and Transport Model (PRZM) 40
3.2.2 Enhancements to PRZM 41
3.3.3 Mathematical Description of the Terrestrial Fate and Transport Processes 43
3.3 Plant Growth Module (PLTGRN) 72
3.3.1 Introduction 72
3.3.2 Development of TEEAM Plant Growth Module as Adapted from EPIC 73

Page
3.3.3 EPIC Modifications for Inclusion in TEEAM 76
3.4 Plant Contamination Transport Module (PLTRNS) 78
3.4.1 Introduction 78
3.4.2 Background 79
3.4.3 Development of Module 79
3.5 Terrestrial Animal Exposure Mpdule 84
3.5.1 Introduction 84
3.5.2 Module Development 85
3.6 The Monte Carlo Module (MC) 95
3.6.1 Description of Monte Carlo Parameter Distributions. 97
3.6.2 Uncertainty in Correlated Variables 99
3.6.3 Generation of Random Numbers 102
4.0 Model Installation and Execution 103
4.1 IBM-PC Compatible Environment Requirements 103
4.1.1 Hardware 103
4.1.2 Software 103
4.2 Loading Executable Codes and Test Data Files 104
4.2.1 Executing Test Data Inputs 105
4.2.2 Verifying Test Data Outputs 105
4.3 General Procedures for TEEAM Execution 105
4.4 Machine and Compiler Dependencies 106
5.0 Input Sequence Development 108
5.1 Overview of TEEAM Input Data 108
5.2 Description of Input Files for TEEAM Modules 109
5.2.1 Execution Supervisor 109
5.2.2 Input Data for the FSCBG Module 111
5.2.3 Input Data for the Spray Grid Definition Module 112
5.2.4 Input Data for the Terrestrial Fate and Transport Module 113
5.2.5 Plant Growth and Translocation Location Modules 115
5.2.6 Input Data for the Terrestrial Animal Exposure Module 116
5.2.7 Input Data for the Monte Carlo Module 117
6.0 Parameter Estimation 179
6.1 Introduction 179
6.2 FSCBG Parameters 179
6.2.1 Aerial Spray Application 180
6.2.2 Ground Spray Application 187
6.3 GRDDEP Parameters 190
6.4 TFAT Parameters 191
6.4.1 Original PRZM Parameters 191
6.4.2 Infiltration and Ponding 238
6.4.3 Volatilization and Pond Chemistry 241
6.4.4 Granular Formulations 242
6.4.5 Soil Surface Temperature Regression Coefficients 245
6.5 PLTGRN Parameters 245
6.6 PLTRNS Module 246
6.6.1 RW--Root Reflection Coefficient 246

Page
6.6.2 LAMBDA--Degradation Rate of the Contaminant Within the Plant 247
6.6.3 KOW--Octanol-Water Partition Coefficient 248
6.6.4 KP--Partition Coefficient 249
6.6.5 RHONA--Ratio of Dry Weight to Wet Weight 249
6.7 APUM Module 249
6.7.1 Species Abundance 249
6.7.2 Animal Movement 251
6.7.3 Feeding, Uptake, and Depuration 253
6.8 Sensitivity of TEEAM to Input Parameters 263
6.8.1 Sensitivity Analysis Approach 264
6.8.2 Sensitivity Analysis Results 264

7.0 Model Output 269

7.1 Introduction 269
7.2 INPREA 269
7.3 FSCBG 269
7.4 TFAT 269
7.5 APUM 276
7.6 MCARLO 282

8.0 Example Application 287

8.1 General Problem Setting 287
8.2 FSCBG and GRDDEF Inputs 287
8.3 TFAT Inputs 288
8.4 PLTGRN and PLTRNS Inputs 288
8.5 APUM Inputs 288
8.6 TEEAM Simulation Results 289

9.0 Model Architecture 294

9.1 Code Architecture 294
9.1.1 Pesticide Application/Deposition 297
9.1.2 Terrestrial Fate and Transport 302
9.1.3 Plant Growth 304
9.1.4 Plant Contaminant Transport 305
9.1.5 Terrestrial Animal Exposure 305
9.1.6 Monte Carlo Simulation 306
9.2 Intermodule Communication 308
9.3 Coding Conventions 308
9.4 File Utilization 308

10.0 Simple Models for Predicting Toxicant Accumulation in Terrestrial Wildlife: ATTEAM 324
10.1 Model Description 324
10.1.1 Model 1. Single Toxicant Application with First-Order Soil Decay 324
10.1.2 Model 2. Continuous Toxicant Application with First-Order Decay 327
10.1.3 Model 3. Steady-State Concentrations under Continuous Deposition 327
10.2 Solution of Model Equations 327

Page
10.3 Model Acquisition, Installation, and Execution 330
10.3.1 Hardware 331
10.3.2 Software 331
10.3.3 Installation and Execution Instructions 331
10.4 Model Input Sequence Development 332
10.4.1 Input Parameter Description 332
10.4.2 Batch Input Sequence 336
10.4.3 Interactive Input 337
10.5 Parameter Estimation 341
10.5.1 Mass Estimates 344
10.5.2 Rate Constants 345
10.5.3 Initial Pesticide Concentrations 347
10.5.4 Estimation of Parameters for Monte Carlo Analysis 347
10.6 Output Files 350
10.7 Example Problem 352
11.0 References 356
Appendix. ATTEAM Example Output using Default Parameter Values . . 366

LIST OF TABLES

Number		Page
5-1	Input formats for theexecution supervision module (EXESUP)	120
5-2a	Input formats for FSCBG module	124
5-2b	Explanation of FSCBG options (ISW values)	137
5-3	Input formats for the spray grid definition module	140
5-4	Input formats for the TFAT meteorology file	143
5-5	Input formats for the terrestrial fate and transport module (TFAT)	144
5-6	Variable designations for TFAT time series file	157
5-7	Input formats for the plant growth (PLTGRN) and plant translocation (PLTRNS) modules	159
5-8	Input formats for the terrestrial animal exposure module (APUM) .	164
5-9	Input formats for the Monte Carlo module (MC)	171
5-10	PNAME labels used to identify Monte Carlo input variables	174
5-11	SNAME labels used to identify Monte Carlo output variables . . .	176
6-1	FSCBG parameter specifications for four meteorological regimes .	181
6-2	Aircraft-specific model parameters	183
6-3	Typical FSCBG spray drop size distribution parameters	184
6-4	Spray drop size range, approximate recovery rate, and recommended use of various spray nozzle types	185
6-5	Drop size distribution of aerosols and sprays, cumulative percent by volume	186
6-6	Actual daytime hours for latitudes 24° to 50° north of equator .	195
6-7	Indications of the general magnitude of the soil/erodibility factor, K	197
6-8	Values of the erosion equation's topographic factor, LS, for specified combinations of slope length and steepness	198
6-9	Values of support-practice factor, P	199
6-10	Generalized values of the cover and management factor,C, in the 37 states east of the Rocky Mountains	200
6-11	Interception storage for major crops	203
6-12	Agronomic data for major agricultural crops in the United States	204

Number Page

6-13 Runoff curve numbers for hydrologic soil-cover complexes 205

6-14 Method for converting crop yields to residue 206

6-15 Residue remaining from tillage operations 206

6-16 Reduction in runoff curve numbers caused by conservation tillage and residue management 207

6-17 Values for estimating WFMAX in exponential foliar model 208

6-18 Pesticide soil application methods and distribution 213

6-19 Degradation rate constants of selected pesticides on foliage . 215

6-20 Physical characteristics of selected pesticides for use in development of partition coefficients (using water solubility) and reported degradation rate constants in soil root zone 217

6-21 Octanol water distribution coefficients and soil degradation rate constants for selected chemicals 222

6-22 Coefficients for linear regression equations for prediction of soil water contents at specific matric potentials 227

6-23 Hydrologic properties by soil texture 230

6-24 Descriptive statistics and distribution model for field capacity (percent by volume) 231

6-25 Descriptive statistics and distribution model for wilting point (percent by volume) 232

6-26 Mean bulk density for five soil textural classifications 234

6-27 Descriptive statistics for bulk density 235

6-28 Descriptive statistics and distribution model for organic matter 236

6-29 Representative saturated hydraulic conductivity ranges for sedimentary materials 238

6-30 Values of Green-Ampt parameters for SCS hydrologic soil groups . 239

6-31 Descriptive statistics for saturated hydraulic conductivity . . 240

6-32 Estimated values of Henry's constant for selected pesticides . . 243

6-33 Measured rate constants for release of pesticides from granules. 244

6-34 Example regressions of surface soil temperature on air temperature 246

6-35 Plant growth parameters, typical ranges 247

6-36 Plant growth parameters, crop specific values 248

6-37 Examples of microphytic feeders and of carnivores that act as secondary and tertiary consumers within or on top of the soil . 251

6-38 Populations of earthworms in different habitats 252

Number Page

6-39 Use of various habitats by mallard ducks in Nebraska 253

6-40 Food intake rates and assimilation efficiencies for various common soil-dwelling organisms 255

6-41 Proportion by volume of plant and animal foods in the esophagi of mallards collected during breeding seasons of 1974-80 in south central North Dakota 258

6-42 Depuration rates for various pesticides in various animal species found in the literature 260

6-43 Input parameters used in sensitivity analyses and their assumed distribution properties 265

6-44 Significant parameters controlling pesticide dosage to the target species 267

6-45 Significant parameters controlling pesticide concentrations in the target species 267

9-1 List of subroutines by module and description of their functions 310

9-2 Common block names, topics, and include file names 319

9-3 Parameter statements, parameter definitions, and include file names 320

10-1 Default values for ATTEAM model control parameters 334

10-2 Defalut values for system descriptive parameters 335

10-3 Formats for batch input file 337

LIST OF FIGURES

Number Page

2.1 Ecosystem components and intercompartmental transfer processes (soil/water/atmosphere/plant system) simulated by TEEAM 10

2.2 Ecosystem components and intercompartmental transfer processes (faunal system) simulated by TEEAM 11

2.3 Spatial structure of terrestrial exposure model 14

2.4 Schematic of an ecosystem food chain 16

3.1 Schematic diagram showing geometry used in constructing the distance x_r and effective source height H' for the case when the settling velocity in the jth size category at height $H(V_j;H)$ is less than ω 27

3.2 Schematic plan view showing the line source geometry with respect to a calculation point at $R(\varepsilon,\delta,z)$ for a wind direction θ 29

3.3 PRZM, release 1, model components 41

3.4 Schematic representation of a TFAT module soil layer 45

3.5 SCS trapezoidal runoff hydrograph 59

3.6 Chemical transport and fate in ponded water 61

3.7 Leaf area index as function of above ground biomass minus yield 74

3.8 Cover as function of leaf area index 78

3.9 Schematic of plant contaminant transport module (PLTRNS 80

5.1 Sample execution supervisor input data file (TMRUN.DAT) 110

6.1 Pan evaporation correction factors 193

6.2 Diagram for estimating soil evaporation loss 194

6.3 Diagram for estimating SCS soil hydrologic groups 209

6.4 1/3-Bar soil moisture by volume 228

6.5 15-Bar soil moisture by volume 229

6.6 Mineral bulk density 233

6.7 Estimation of drainage rate AD versus number of compartments . . 237

6.8 Correlation matrix used in the sensitivity analyses 266

7.1 Example of a portion of the TFAT input echo 270

7.2 Example of the PLTGRN/PLTRNS input echo 271

Number Page

7.3 Example of a portion of the APUM input echo 272
7.4 Example of a portion of the GRDDEF input echo 273
7.5a Example of the FSCBG input echo 274
7.5b Example of the FSCBG output 275
7.6 Example of habitat hydrologic status output 277
7.7 Examples of the habitat pesticide mass status output 278
7.8 Example of the habitat pesticide concentration output 279
7.9 Example of the habitat time source output 280
7.10 APUM dosage breakdown output file 281
7.11 APUM time series output file 282
7.12 Monte Carlo cummary output file 283
7.13 Monte Carlo parameters output file 286
8.1 TEEAM output for the example application 290
9.1 TEEAM main program structure 296
9.2 Batch input module (BATENT) structure 297
9.3 Executive supervisor (EXESUP) structure 298
9.4 TEEAMAIN program structure 299
9.5 Module FSCBG structure 301
9.6 Module TFAT structure 303
9.7 Module PLTGRN structure 304
9.8 Module PLTRNS structure 305
9.9 Module APUM structure 306
9.10 Module MCARLO structure 307
9.11 FSCBG linkage to TEEAM habitats 309
10.1 Schematic of ATEEAM model structure 325
10.2 Screen 1 ATEEAM model title screen 338
10.3 Screens 2, 3, and 4 from ATEEAM model 339
10.4 Screens 5 and 6 from ATEEAM model 340
10.5 Screens 7 and 8 from ATEEAM model running in interactive mode . 342
10.6 Screens 9 and 10 from running ATEEAM model in interactive mode . 343
10.7 Example of MCARLO.OUT output file 350
10.8 Example of TLEV1.OUT output file when model is run in Monte Carlo mode 351

Number Page

10.9 Example of TLEVL.OUT output file when model is run in deterministic mode 352

10.10 Example of histogram printer plot found in user-specified output file 353

10.11 Example of CDF printer plot found in user-specified output file . 354

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SECTION 1

INTRODUCTION

1.1 BACKGROUND

The U.S. Environmental Protection Agency is continually faced with issues concerning the regulation, restriction, or banning of chemical substances. Decisions concerning these chemicals are based upon the concept that humans or animals may be subjected to concentrations of chemicals through various routes of exposure. In the case of humans, chemicals are normally subject to restrictions upon their use if the sum of the loadings from these various routes exceeds an acceptable intake level (ADI, RFD). Until now, the Agency has had no computer-based methodology for calculating exposures to terrestrial animals to compare to existing toxicological data. Data on wildlife contamination levels and reports of wildlife kills from pesticide use indicate that the impact of these exposures is substantial (RSPB 1965; DeWeese et al. 1986).

Most pesticides are registered for use in terrestrial environments. Other xenobiotics are released to the atmosphere and are subsequently deposited on soil and plant surfaces, where they are subject to cycling in terrestrial ecosystems, providing exposures to plants and animals. Little is known concerning the magnitude of exposures among the various exposure pathways. Generation of this information requires simultaneous simulation of environmental concentrations in food items and the intake of contaminants via the food chain and other exposure pathways to the species of interest.

In order to establish risk, probabilities of various levels of exposure must be made utilizing the model. This requires that variations in naturally occurring processes which serve to cycle xenobiotics through the terrestrial ecosystem and the uncertainty in model parameters be considered, as well as the impact of management strategies. All of these factors have direct implications for risk analysis and risk management.

1.2 OBJECTIVES AND SCOPE

The objective of this model development effort was to build a simulation model which can be used by the Agency to evaluate the magnitude of exposure from organic toxicants to plants and animals in terrestrial ecosystems. The simulation of events occurring in a terrestrial ecosystem which affect chemical exposure to plants and animals is a complex problem because the interactions which occur in such systems are complex. Ecosystems are characterized by an intricate web of feedback mechanisms which keep the ecosystem in balance. Many varied processes may affect this balance.

It was not possible, in this model development effort, to account for all of these processes or their effects. Therefore, a number of limitations to the scope of the development effort were necessary. These are discussed in the following sections under the following categories:

- Long-Term Ecological Changes
- Short-Term Toxicant-Induced Ecosystem Changes
- Typical Model Applications
- Priority Ecosystems
- Outputs of Interest
- Chemical Release Scenarios

1.2.1 Long-Term Ecological Changes

Some ecological processes operate over long periods of time (e.g., forest succession) and may be due to internal changes (for instance, in nutrient balances) or external changes (e.g., climate). It was beyond the scope of this modeling effort to consider these types of changes. Furthermore, it is probably inappropriate to consider them within the context of this work. The history of organic chemical production extends back several decades. The useful life of most chemicals encompasses relatively short periods of time due to continual advances in technology. In addition, the persistence of organic chemicals in the environment is relatively short compared to ecosystem changes of the type mentioned above.

1.2.2 Short-Term Toxicant-Induced Ecosystem Changes

Of greater pertinence to this work are ecosystem perturbations which might be caused by toxicant insult. There is little evidence to demonstrate that toxicants produce effects of such significance to cause terrestrial ecosystems to shift to new equilibrium points. This supposition is supported by the recent work such as that of Biederbeck et al. (1987) and Baker et al. (1986). However, toxicant insult may have important short-term effects which may dramatically affect exposure to species of interest. For instance, the toxicant might temporarily reduce the population of the primary food item of the species of interest. This species, then, might

- Leave, seeking a new source of this food item

- Switch to an alternative food source, thereby decreasing exposure

- Switch to an alternative food source, increasing exposure

- Prey on the contaminated, reduced population, resulting in the species' own sickness or death

In general, the toxicant effects which might affect exposures can be broken down into two broad categories:

- Avoidance/attraction

- Loss of habitat

Avoidance/attraction behavior can be direct or secondary. Direct effects would be repulsion or attraction to the chemical itself. A secondary response would be, for instance, a repulsion or attraction to prey which had been weakened by exposure to the toxicant. There is research currently underway to investigate the avoidance/attraction behavior exhibited by various species in response to a variety of chemicals and various formulations of those chemicals. However, at this time, this information cannot be generalized among species, chemicals, or formulations so that avoidance/attractance mechanisms cannot be modeled realistically. However, this is definitely an area in which further development of the model is warranted as understanding of the processes advances.

Loss of habitat can be subdivided into several effects. Loss of nesting habitat could occur due to spraying of an herbicide, directly destroying cover or other characteristics of the nesting site. Loss of feeding habitat could result due to mortality or other loss of preferred food items, such as failure of reproduction in lower trophic level fauna or failure of fruit production in plants. Although the impact of these effects on wildlife exposures to chemicals is probably substantial, the cause and effect relationships that govern the relationships between loss of habitat and behavioral responses of specific species are not generalizable. For many species, habitat requirements have not even to date been well documented.

Therefore, it is felt that simulation of complex sequences of behavioral responses resulting from toxicant insult is not possible at this time. An important assumption which derives from this conclusion is:

- Toxicants do not affect the state of the ecosystem. These characteristics which describe the "state" include:

  - population levels of animals (birth, death rates)

- assemblage of species in the plant community
- behavior of animals (migration, feeding, etc.)

Collectively, these assumptions require that the ecosystem is at a point of equilibrium which will be user defined at the outset of the simulation and will not change over the simulation period. In essence, then, TEEAM is an exposure model in the setting of a terrestrial ecosystem, and not an ecosystem model which can account for the effects of toxicants on the ecological state of the system.

1.2.3 Typical Model Applications

The model is expected to be used by the Environmental Protection Agency as a regulatory tool. The utility of the model is to aid in the formulation of strategies for mitigating damage to "terrestrial ecological systems" based upon model simulation output. This requires that the model be capable of simulating exposure to terrestrial plant or animal species of interest and that the impact of regulatory decisions on exposures can be estimated by the model. Regulatory strategies for pesticides might include:

- Banning
- Restriction of application rates
- Restriction on the timing of applications
- Restriction of application in or within certain distances of sensitive ecosystems
- Restriction on certain types of chemical formulations
- Restriction on the cumulative quantity of a chemical which could be applied in the same ecosystem over a given time period

The model has been constructed with the capability to address these strategies. Furthermore, the model is designed to be applied to simulate a generalized ecosystem. For instance, the model might be applied to evaluate exposure to sage grouse in wheat field ecosystems in the northern Great Plains. It would not likely be applied to a specific field in a specific township, range, etc. Therefore, the need for the capability to simulate on a high level of spatial detail is deemed unnecessary.

Obviously, since the model is to be utilized for risk management, probabilities of events must be generated by the model as well as the events themselves. This requires a framework by which these probabilities can be generated. Therefore, the typical model application may involve the use of the Monte Carlo simulation capability.

1.2.4 Priority Ecosystems

There are a number of ecosystems which are of potential interest to the Agency. Certainly ecosystems in which the regulation of chemicals may have a large economic impact are of concern. Other less economically important ecosystems which might contain endangered or threatened species may also be of concern. It seemed unnecessary to prespecify ecosystems in which the Agency has an interest for the purpose of the model development effort, and this was not done. To some extent, this may have aided in the development of a more generalized approach. However, at this point in time the model focuses on avians in agricultural ecosystems with pesticides as the toxicant of greatest concern. It is possible, through judicious selection of parameters, that forest ecosystems may be simulated. However, simulation of ecosystems such as wetlands on tidal marshes is clearly beyond the scope of the current model.

1.2.5 Outputs of Interest

The most important question concerning model output is that of relevant toxicological endpoints. These endpoints might include:

- Death of species of interest
- Some measure of health of the population or an individual or population of the species (e.g., reproductive failure, egg shell thinning)
- Behavioral modifications (e.g. nonphysical effects)

Since most of the toxicological information available on the effects of pesticides or xenobiotics on animals is in the form of a lethal dose (e.g., LD_{50}, LD_{10}), the output of interest is most likely the dosage (through time or cumulative) to the species of interest. Because deciding upon mitigation strategies may involve looking at major pathways of exposure, it was also thought to be desirable to be able to view the total dosage in terms of its components (e.g., inhalation, ingestion, absorption) or to further categorize into concentrations and food/air/water intake rates. This implies that tissue burden in plants or animals in lower levels of the trophic systems, in the soil, water, and air, are also important outputs.

Other effects may ultimately be simulated based upon concentrations in plants and animals (e.g., avoidance/attraction behavior). At some point, it may be desirable to have the capability to simulate and/or output concentrations in various organs of the plants or animals in order to determine certain effects of the toxicant's presence. However, this has not been implemented in the current version of model.

1.2.6 Chemical Release Scenarios

The terrestrial ecosystem exposure model was formulated for use by both the Office of Pesticide Programs (OPP) and the Office of Toxic Substances (OTS). Therefore, there was a desire to address pesticides as well as other xenobiotics. Once the chemical is placed into the ecosystem, it is postulated that the processes involved in cycling of organic toxicants are no different. Therefore, the key difference in terms of modeling pesticides versus xenobiotics is the application/deposition process. Pesticides are released to terrestrial environments for the most part in ground or aerial spraying events, either to bare soil and/or to plant canopies. Application may also take the form of soil injection or application in irrigation waters (chemigation). Irrigation may take on various forms (spraying, flooding, drip, etc.). Toxics other than pesticides, with the exception of spills, are almost entirely deposited from atmospheric sources. Deposition may occur in the form of gases, dissolved in precipitation or adsorbed to particulate matter. Since the initial focus of this modeling effort is on pesticides, the modeling of aerial or ground spray deposition events is addressed in this report rather than toxicant deposition modeling from atmospheric sources. Chemigation is not addressed by the model.

1.3 REPORT ORGANIZATION

This report is divided into 10 major sections inclusive of this introduction. Sections 2 and 3 provide documentation of the content of the model. Section 2 is an overview and Section 3 describes model theory, algorithms, and solutions to equations in detail.

Sections 4 through 8 form a model user's guide. Section 4 contains information on model installation and execution; Section 5, input sequence development; Section 6, parameter estimation Guidance; Section 7, a description of model output; and Section 8, some example model applications.

Section 9 constitutes the model programmer's guide. It contains information on model structure, coding conventions, intermodule communication and file manipulation.

Section 10 describes a simplified analytical food chain exposure model (A-TEEAM). The discussion includes theory, solution of equations, user's guidance, and example problems.

SECTION 2

MODEL OVERVIEW

The purpose of this section is to give an overview of the model in its current state of development. This level of detail should suffice for those readers who are not interested in the more mathematical descriptions contained in Section 3. In evaluating the appropriateness of this model development effort it is important to keep in mind the objectives and scope discussed in Section 1. It is anticipated that the model will continue to evolve. Therefore, the model has been built in a modular style. In addition, "hooks" (that is, interfaces) have been left in places to facilitate the addition of pieces of software at a later date. Because of this, model capabilities may seem incomplete to some reviewers, or an analyst of the code may notice that certain calculations are performed and not subsequently used. It is hoped that the majority of these occurences have, in fact, been planned, and will not interfere with the application of the current version of the code.

This section begins with a brief review of some previous terrestrial ecosystem-type exposure assessment modeling to indicate the state-of-the-art. It then overviews the features and limitations of the current model and concludes with recommendations for continued development.

2.1 PREVIOUS WORK

Historically, exposure modeling in support of risk assessment for organic toxicants has concentrated on aquatic exposure resulting either from transport from the terrestrial system (e.g., due to runoff) or direct discharge (e.g., toxics in wastewater effluents). Notable examples of modeling procedures which provide this capability include HSPF (Johanson et al. 1980), TOXIWASP (Ambrose et al. 1983), EXAMS (Burns et al. 1982), and SWRRB-EXAMSII (Offutt, personal communication). The same general approach for toxics was adopted by OTS with models developed for generalized multimedia analyses. UTM-TOX (Patterson et al. 1984) and TOXSCREEN (Hetrich and McDowell-Boyer 1984) simulate the transport and fate of toxicants from their sources through the air and their deposition on the land or through forested watersheds and idealized urban environments, respectively. All the above referenced models treat the terrestrial environment as a source or a sink. Spatial distribution within the terrestrial environment and concentration profiles for ecologically important compartments (e.g., plants and other wildlife food sources) are largely ignored in these models. However, with some modifications, such models could feasibly have been used as a framework on which to develop a terrestrial ecosystem exposure assessment model.

Some limited work has been done in the past several years to address the problem of estimating chemical exposures in terrestrial ecosystems. A program called FEAST (Kiekebusch et al. 1981) was developed to evaluate exposures to humans by tracing toxicant movement through soil, uptake by plants and livestock, and food processing. A similar model, GEOTOX, was recently developed which provides the same type of capability, although it is more refined (McKone and Layton 1986). GEOTOX is a compartmental, multimedia model which investigates the fate and transport of organic toxicants in air, soil, water, and human food products, and evaluates health effects. The model solves a set of differential equations (one for each compartment) either for steady state or time varying applications. The code also evaluates mass transfer coefficients for the advection and diffusion processes which are assumed to move contaminants between compartments. Process descriptions are kept extremely simple, consistent with the screening-level application intended for the model.

Another model called PATHWAY (Kirchner and Whicker 1984) simulates the transport of radionuclides in agroecosystems and ultimate exposure to humans. PATHWAY is a dynamic continuous simulation model and has been validated with historical data on toxicant fallout and uptake into vegetation and livestock. As for FEAST and GEOTOX, the focus of this model is human exposure as opposed to wildlife.

In 1984, a modeling effort was undertaken to evaluate exposure of pesticides to ducks and upland game birds in wheat field ecosystems. The model made use of PRZM (the Pesticide Root Zone Model) (Carsel et al. 1984) to describe the fate and transport of pesticides in the soil and the FSCBG model (Dumbauld, Bjorklund, and Saterlie 1980) to describe application/deposition and drift during aerial spraying events. Elementary soil arthropod and plant uptake and translocation models were added to PRZM in order to simulate pesticide concentrations in the food items of these avian species. The approach is fully described in Dean et al. (1984), and various components are described in Donigian and Dean (1985). This work has been utilized as a building block for the current model development effort.

Recommendations for additional capabilities needed for simulation of exposure in a generalized terrestrial ecosystem were made as a result of the above mentioned modeling effort. They included:

- A more accurate description of partitioning of pesticide between foliage and soil during the spray events, accommodating different types of sprayers, leaf and plant geometry

- A submodel to describe foliar absorption and translocation into the plant

- Simulation of organisms on plant foliage and toxicant uptake by these organisms

- The addition of types of soil organisms other than macroarthropods (for example, oligochaetes) and descriptions of organism growth and mortality dynamics in lieu of assuming a fixed population

- Food chain dynamics and biomagnification (prey/predator relationships)

Some of these recommendations have been incorporated as components of the TEEAM code, described below.

2.2 MODEL FEATURES

The utility of a piece of software can be judged by its ease of application in the opinion of the user and its appropriateness to solving the problem at hand. The model has been conceived with both of these factors in mind. In the following sections, the processes simulated, the model's spatial and temporal structure, and user-oriented features of the software are discussed.

2.2.1 Processes Simulated

In order to realistically simulate exposure to plants and animals in terrestrial ecosystems, the model contains the following simulation capabilities:

- Toxicant application/deposition
- Soil/atmosphere fate and transport
- Plant uptake, fate, and translocation
- Terrestrial food chain bioaccumulation and biomagnification

Figures 2.1 and 2.2 show a schematic overview of the processes which the model simulates.

Figure 2.1 overviews the processes involved in the soil/plant/atmosphere system. The toxicant is deposited in an application event, or to either plant or soil surfaces. Drift into non-target areas can be quantified by using the FSCBG module. FSCBG is an analytical model which simulates spray deposition from an elevated line source. Currently, exposure to animals (inhalation, dermal contact, etc.) during spray events is not simulated. Deposition is allowed to occur to various user-specified levels within the canopy, although this information is not used in the current version of the model. The application event may be either aerial or ground spraying, in which case drift to adjacent habitats may be quantified. Ground spraying events are simulated by manipulating certain parameters of the aerial spray model, as described in Section 6. Foliar, soil surface, and soil subsurface applications are also addressed. Application/deposition due to toxicant fallout and chemigation are not simulated at this time. Toxicants may be applied in granular form from which they may slowly be released into the soil or be consumed directly by terrestrial animals. Application in the form of treated seeds may also be simulated.

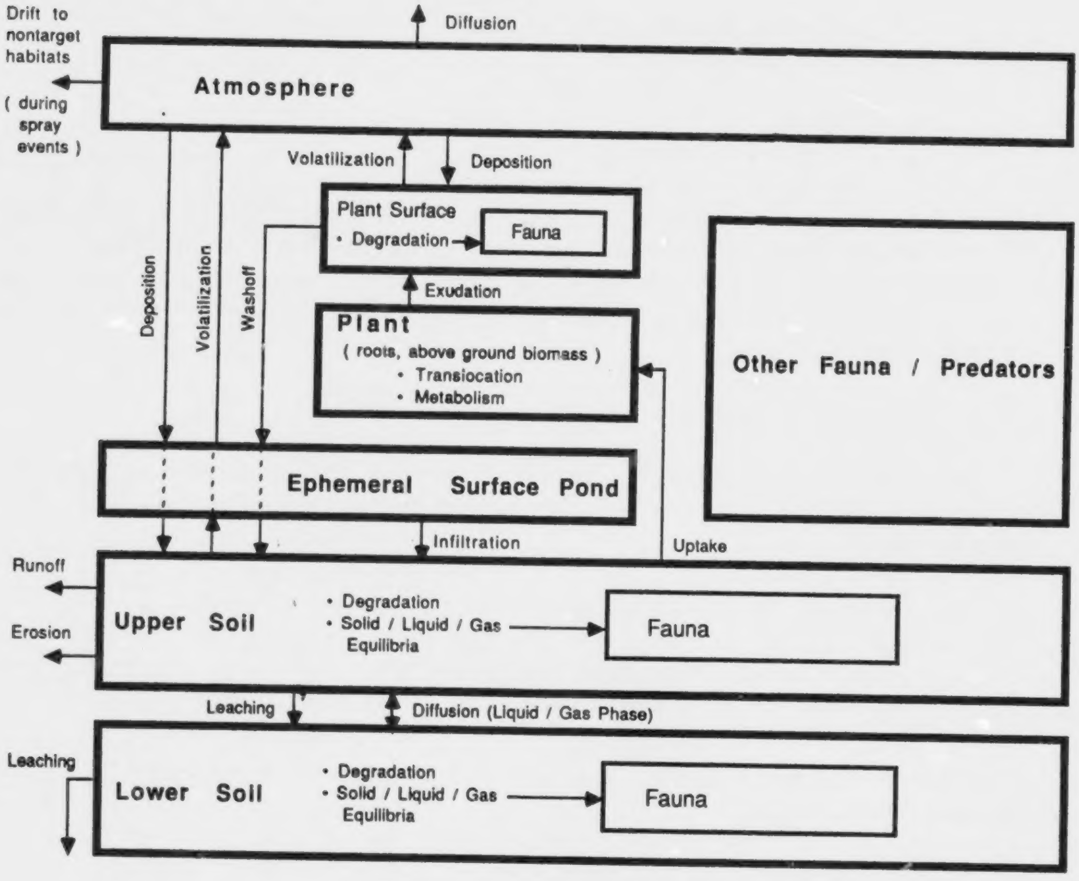

Drift to nontarget habitats (during spray events)
Diffusion
Atmosphere
Volatilization
Deposition
Plant Surface
• Degradation
Fauna
Exudation
Plant
(roots, above ground biomass)
• Translocation
• Metabolism
Deposition
Volatilization
Washoff
Other Fauna / Predators
Ephemeral Surface Pond
Infiltration
Uptake
Runoff
Erosion
Upper Soil
• Degradation
• Solid / Liquid / Gas Equilibria
Fauna
Leaching
Diffusion (Liquid / Gas Phase)
Leaching
Lower Soil
• Degradation
• Solid / Liquid / Gas Equilibria
Fauna

Figure 2.1 Ecosystem components and intercompartmental transfer processes (soil/water/atmosphere/plant system) simulated by TEEAM.

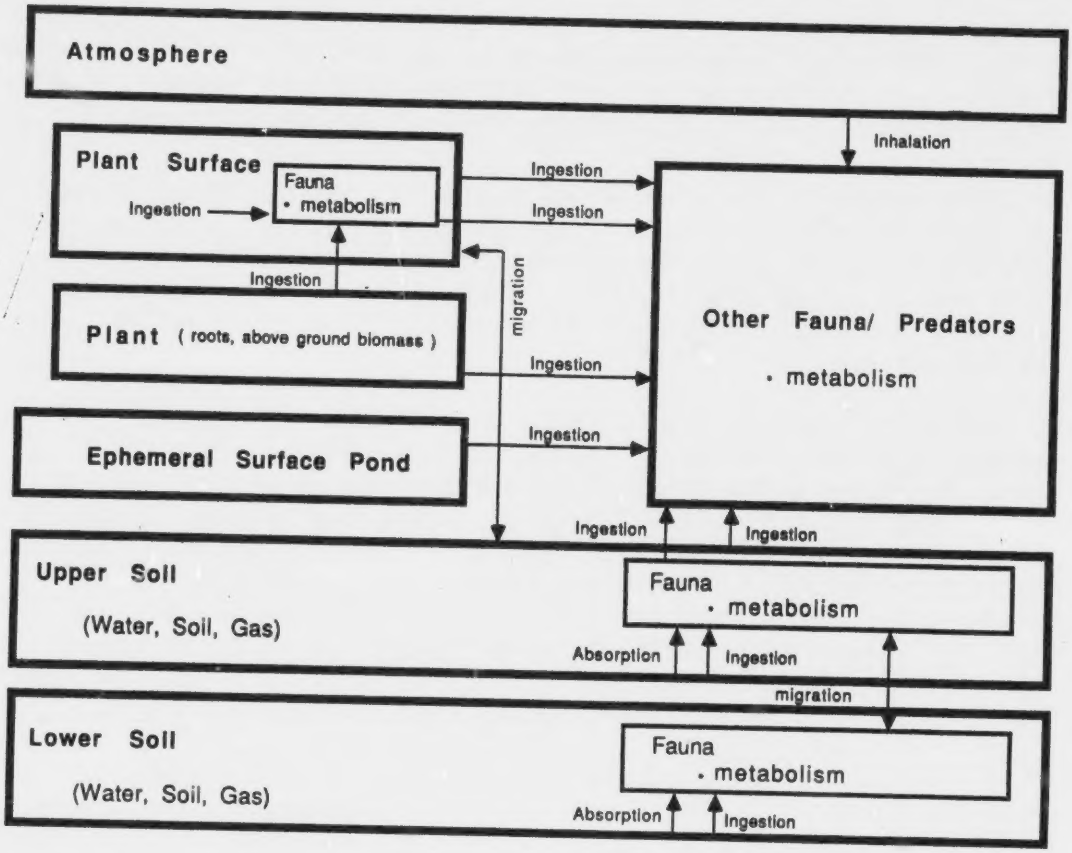

Atmosphere
Inhalation
Plant Surface
Fauna
• metabolism
Ingestion
Ingestion
Ingestion
Ingestion
migration
Plant (roots, above ground biomass)
Ingestion
Other Fauna/ Predators
• metabolism
Ephemeral Surface Pond
Ingestion
Ingestion
Ingestion
Upper Soil
(Water, Soil, Gas)
Fauna
• metabolism
Absorption
Ingestion
migration
Lower Soil
(Water, Soil, Gas)
Fauna
• metabolism
Absorption
Ingestion

Figure 2.2 Ecosystem components and intercompartmental transfer processes (faunal system) simulated by TEEAM.

Terrestrial fate and transport calculations are made using a modified version of the PRZM code. Toxicants deposited on plant surfaces may be washed off during rainfall events and moved to the soil surface, returned to the atmosphere via volatilization, or degraded on the plant surface. Foliar absorption and subsequent translocation throughout the plant are not currently simulated.

Toxicants on the soil surface or in the soil may be present in adsorbed, dissolved, or gaseous phases. Phase concentrations are determined assuming equilibrium among phases and making use of adsorption partition coefficients and Henry's Law constants. Toxicants in the upper soil may subsequently be leached into the lower soil, degraded, taken up by plants, returned to the atmosphere via volatilization, or lost to the system through erosion by water and runoff. Similar processes operate in the lower soil profile (below the root zone) with the exception of plant uptake. Throughout the soil, transport occurs due to advection, dispersion, and liquid and gas phase diffusion. Following precipitation events, water may be temporarily ponded at the soil surface. Various chemical fate processes may act upon the chemical within the pond, including volatilization, degradation, and infiltration into the soil.

An adaptation of the plant growth module from the EPIC model is used for simulation of plant growth. Plant growth affects the concentration of pesticide within the plant and micrometeorological processes which control spray deposition and volatilization. Plant uptake is controlled by the rate of evapotranspiration, chemical adsorption in soil, and reflection at the root surface.

Within the plant, toxicants are partitioned between roots and aboveground biomass and may be degraded while traveling through the plant. Advection of the chemical through the plant is modified via partitioning into the nonaqueous phase. Chemicals which travel completely through the plant are exuded back into the atmosphere. Currently, this exuded quantity exits the ecosystem and does not contribute to concentrations within the plant canopy. In the atmosphere within the plant canopy, various degradation processes may serve to diminish the chemical mass. In this model, the chemical mass is removed from the system only by diffusion into the atmosphere above the plant canopy height.

The soil, water, air, and plants in the terrestrial system provide vectors for uptake of pesticides by animals. TEEAM computes the dosages to, as well as concentration in, the biomass of the modeled species. The components of the faunal system and associated transfer processes are shown in Figure 2.2. In general, animals may be present in or on the soil and depending upon their physiological capabilities and behavior, they may migrate between various layers in the soil. They may also migrate between ecosystem habitats as described in the next section. Soil fauna may feed on organic detritus, microbes (bacteria) in the lower trophic levels and on earthworms, arthropods, crustaceans, molluscs, and the like in higher trophic levels. Animals may also consume living above ground plant biomass. They may also absorb chemicals from the soil system, bioconcentrating them in their tissues. Animal mortality and the return of toxicants to the soil in this manner is not simulated. Biomass levels of each of the modeled species are assumed to be fixed for a given simulation. It is also the case that the uptake terms in the animal exposure model do not have equivalent sink terms in the terrestrial model. Therefore, the effects of removal of pesticide by animals from the terrestrial system are not accounted for. This should not be a major problem as the amount of chemical residing in the animal biomass is probably small compared to the total amount of chemical in the system.

Higher trophic level predators are also considered. These would be the species of interest to the exposure assessment and may ultimately include various higher level terrestrial herbivores, carnivores, and avians. However, as stated earlier, the model is focused at this time on avians.

Mass balances as calculated within the terrestrial fate and transport module, the plant translocation module, and the animal exposure module. Currently, a global mass balance calculation is not performed. However, simulations using the TEEAM code match reasonably well with ATEEAM (See Section 10) simulations, indicating that mass transfers between the terrestrial and animal exposure modules are handled correctly.

The above discussion describes the processes which occur at a single point in the ecosystem. However, due to heterogeneity of the area which this species inhabits, the model must be capable of simulating subareas (habitats) of various types. The model's spatial features are described below.

2.2.2 Model Spatial Features

The spatial structure of the model is a collection of habitats, having a one-dimensional vertical structure as depicted in Figure 2.3. The modeled ecosystem is broken into these habitats because there is some uniqueness about them in the real ecosystem. For instance, habitat 1 may be the agricultural field to which the chemical is applied which may also serve as a feeding habitat for the species of interest. Habitat 2 might be the nesting habitat of a species that feeds primarily in Habitat 1. Habitat 3, on the other hand, might be an area which received drift during the chemical application event, is visited infrequently by the species of interest, and therefore is different, in terms of exposure potential, from habitats 1 or 2.

In general, habitats are differentiated because there are:

- Distinct differences in plant or animal species in various parts of the ecosystem

- Distinct differences in behavior and/or feeding preferences when various animal species are in these various habitats

- Distinct differences in pesticide or toxicant distribution among habitats

Within each habitat, conditions are assumed to be laterally homogeneous. The effect of minor deviations from this assumption can be addressed through the use of Monte Carlo simulation. It is possible to transfer mass between compartments to account for the effects of wind and animal migration;

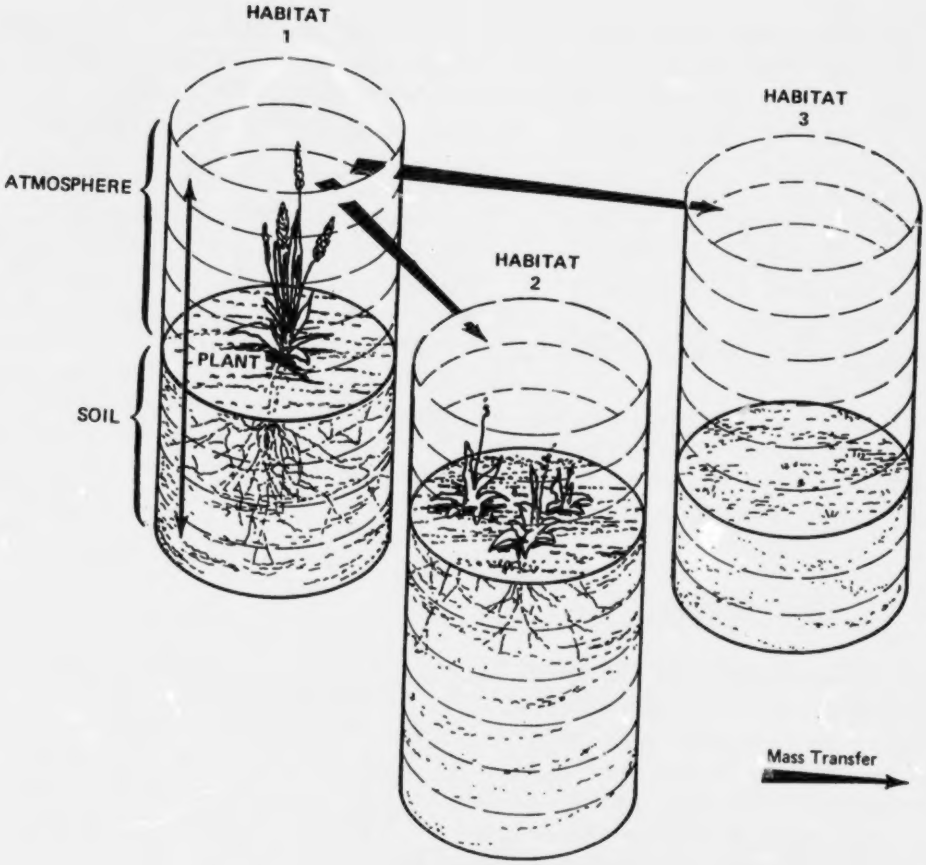


Figure 2.3 Spatial structure of terrestrial exposure model.

however, the dependence of concentrations in a given compartment on the processes occurring in an adjacent compartment is assumed to be weak. Each compartment has a vertical structure, the discretization of which depends upon the dynamics of the processes being simulated. Concentrations in the profile are considered to be strongly dependent upon processes which transfer mass vertically (e.g., volatilization, deposition, percolation of water through the soil, etc.), hence the greater detail in the vertical dimension. As many habitats may be used as are necessary to describe the ecosystem, within the limits of practicality. It is likely that a greater knowledge of the ecosystem will result in greater compartmentalization. Each habitat specified, however, requires a corresponding application of the terrestrial fate model. Since lateral transfers between habitats are assumed to be of relatively minor importance, the order of execution of computations among habitats, is also of little importance. Exact directional relationships between compartments are required by the deposition model to simulate pesticide application events. However, for the operation of the remainder of the modules, exact spatial relationships need not be known.

Animal species are allowed to migrate among habitats. Species in lower trophic levels may be permanent habitat residents, depending upon the area of the habitat selected. As with the differentiation of habitats, as many trophic levels and as many species within each trophic level may be used, as is necessary, to represent the food chain. A schematic of a food chain is shown in Figure 2.4. The food chain also includes plants, soil, and water. The species of primary interest is that in the highest trophic level (1,1).

The boxes in Figure 2.4 represent a single species of interest. In terms of model implementation, however, each box may represent an individual, a group of individuals, or the entire species population within the ecosystem. Thus, each box may be subdivided as necessary to simulate variations among species. For instance, species (3,1) may be present ubiquitously in the soil and relatively immobile. If the ecosystem is spatially segregated into habitats, several subgroups which represent the portion of the community in each habitat would be required. For a species in a higher trophic level, (i.e., species 2,1) a group of several individuals might be simulated. These individuals may or may not be constrained to specific spatial habitats, depending upon their mobility. The range of each species is denoted by specifying habitats that each species is allowed to visit. Thus, the model spatial structure and the trophic structure are integrated. Even though individuals or subpopulations may have the same behavioral tendencies (on the average), a stochastic modeling approach to animal movement and feeding incorporated into the model can be utilized to yield estimates of variability of dosage or body burden of toxicant caused by random movement.

2.2.3 Model Temporal Features

There are several important time-related features of the model which must be pointed out. The model operates in a daily time step. The length of simulation is flexible and can be selected by the model user. For short-lived chemicals which do not accumulate to any great extent in animal tissues, the magnitude of single exposure events to the species of interest is of greatest importance. For less acutely toxic, more lipophilic chemicals, the body burden over the life cycle of the species of interest is of greatest importance. In these cases, the simulation could be as short as a single exposure period (days to weeks) or the species life-cycle (months to years). In other cases, the interest may be in carryover of pesticide from generation-to-generation within the species and/or long-term effects on population levels. In these scenarios, simulation periods of many years may be of interest. The focus of this model is currently short-term lethal exposures; however, longer term simulations may be run. It is recommended that relatively short periods of time be simulated due to the lack of a comprehensive representation of seasonal effects on animals (e.g., behavior, metabolic rates).

Aside from overall simulation length and time step there are other time scale phenomena which are also important. For instance, there may be distinct seasonal or diurnal behavioral patterns in the species of interest. In addition, there may be distinct behavioral differences which are a function of life-cycle stage in the species of interest. Animal behavior (e.g., feeding rates, food preference, movement) is functionally described in the model and governed by sets of user input parameters. For instance, animal movement is simulated using a single lag Markov (autoregressive) process. The process is parameterized by the use of a transition matrix. These such functions themselves do not have seasonal or life-stage effects built into them directly and, currently, there is no way of changing input values to account for seasonal effects.

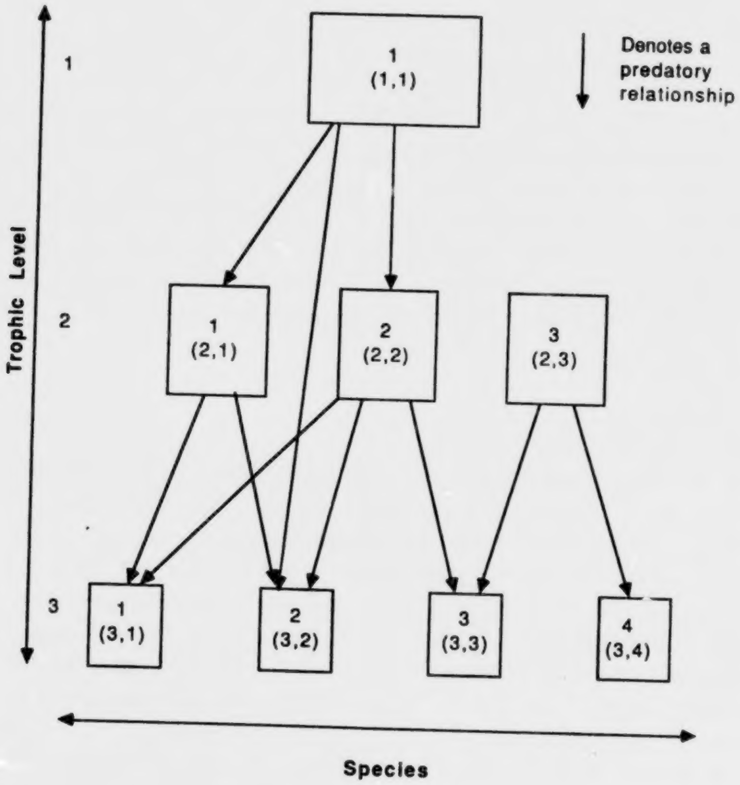


Figure 2.4 Schematic of an ecosystem food chain.

2.2.4 Software Features

Two significant features have been incorporated into the TEEAM model: 1) the ability to simulate multiple habitats, allowing for the simulation of wind drift of an aerial spray applied to one habitat onto an adjacent habitat as well as animal movement among habitats, and 2) a Monte Carlo driver which permits the identification of input parameter uncertainty and which allows the quantification of the uncertainty in selected output parameters.

The TEEAM execution software has been designed for the software user. Extensive error checking and reporting has been incorporated into the software. Most errors are trapped within the software, and an error message displayed to the screen explaining what the error was and where it occurred. If the error is fatal, the program is halted with all files closed permitting the user to examine the files containing input data echo for potentially inappropriate data values. The TEEAM software also has a 'TRACE' option which displays which subroutine the software is currently executing. Thus, if an error does occur, the user will be able to determine the subroutine in which it occurred and the path to that subroutine.

The TEEAM software has been designed to be compatible with the IBM PC compatible microcomputer environment. IBM PC specific features include a screen generator which displays the status of the simulation and time series output files which can be directly imported into popular spreadsheet programs for graphing and analysis. While the software has been designed with microcomputer applications in mind, relatively few changes should be required for adaptation to alternate computer systems. INCLUDE files are used to define array sizes, file unit numbers, and other potentially compiler/computer system-specific parameters. Most, if not all, changes necessary for adaption to alternate computer systems can be accomplished by modifying these INCLUDE files without modifying the FORTRAN code itself.

TEEAM was formed by linking three preexisting computer codes, the Pesticide Root Zone Model (PRZM) (Carsel et al. 1984), and FSCBG (Dumbauld et al. 1980), and plant growth model in EPIC (Williams et al. 1988) to code that was written specifically for this application. As a result, different programming conventions and styles are apparent in the FORTRAN Code. The conventions and style of PRZM and the code written for this project are similar. The most significant contrast in programming conventions and styles are evident between FSCBG and the remainder of the code. No attenpt has been made to either restructure or make cosmetic changes to FSCBG. Neither has any attempt been made to unify input and output styles or formats.

This nonuniformity has both advantages and disadvantages. The advantages are that for users familiar with the preexisting versions of the individual codes, the similarities will be comforting. It is also more apparent, when one is inputting data or reading output, the module to which the input or output belong. Disadvantages include some redundancy, at times, in input, calculations and/or output, and attendant difficulties in interpreting output or debugging/modifying code.

2.3 RECOMMENDATIONS FOR FURTHER WORK

The recommendations for further work with the TEEAM code fall into two categories:

- Additions to existing code and
- Parameter estimation and model verification

2.3.1 Additions to Existing Code

Some additions to the code would augment its ability to realistically simulate toxicant exposures to wildlife. The first recommendation would be to bring the simulation of the animal populations to the same level as that of the plant biomass model. Thus, population models for the species of interest and seasonal effects on animal growth, metabolism, and behavior could be added.

A second recommendation would be to enhance the animal exposure model to simulate chemical fate and transport in various organs of plants and animals. For plants, this might include roots, stems, leaves, seeds, fruit, etc. and for animals, distribution into brain, liver, etc. Along with this might be added other exposure routes. For instance, foliar absorption and translocation could be added for plants, and percutaneous absorption for animals. Although the capability exists within the model to simulate inhalation exposure during spray events, this is not currently available. The adaptations should be made to gain advantage of this capability.

A third category of additions would be the simulation of the effects of the toxicant on the ecosystem. For instance, the effects of growth inhibition of herbicides on certain plants or the effects on seed production might be of concern. Simulation of avoidance/attraction effects of pesticides on food ingestion by animals would significantly improve the capability to accurately simulate exposure.

Two additional extensions would enhance the applicability of the model. One would be the addition of algorithms to simulate the loading of atmospheric toxicants to the terrestrial system. Currently only discrete spray or application "events" can be simulated. A second would be the extension to animals other than avians. This would chiefly be done by giving appropriate parameter guidance for the generalized movement and feeding algorithms already in the model.

2.3.2 Parameter Estimation and Model Verification

The third category of recommendations is in the area of validating and improving, as necessary, the accuracy of the model. Two ways of doing this are improving estimates of input parameters and verifying the model algorithms. This could be done by using a short term (weeks to months) field trial for the current model, looking at acute toxic effects and toxicant concentrations in various media over time. System data would be used to improve parameter estimates through calibration and identify inappropriate process algorithms. It would also be appropriate to parameterize a number of preselected sets of ecosystems in order to facilitate the application of the model for regulatory purposes.

SECTION 3

TEEAM MODULES AND PROCESSES

This section describes the TEEAM modules and details the processes which are simulated by each. Presently, there are six computational modules:

- Toxicant application/deposition
- Soil/atmosphere terrestrial fate and transport
- Plant growth
- Plant contaminant transport
- Terrestrial animal exposure
- Monte Carlo simulation

3.1 TOXICANT APPLICATION/DEPOSITION SUBMODEL

3.1.1 Introduction

A prerequisite to determining the fate of pesticides in the environment and the resulting effects on the ecosystem is the ability to realistically characterize the processes which bring them into the environment at the point of application. This requires knowledge of the methods of application as well as the subsequent transport and deposition processes. The application of pesticides may result in exposure both during and after the spray event. During the event, high concentrations of sprayed material may be inhaled by animal species. Therefore, it is important to predict these concentrations to determine overall exposure. The exposures which occur after the event result from deposition which has occurred to soil or vegetation either within or out of the targeted spraying area. Therefore, both on- and off-site deposition rates are calculated and provided as input to the exposure models.

A variety of application/deposition scenarios are possible. These have been discussed under "Chemical Releases" in Section 1.2.4. In this version of the model, spray application events are assumed to be of central importance. Pesticide spraying methods can be divided into two main categories: (1) aerial applications, and (2) ground-based spray application methods. The aerial spraying technique is widely used and has the greatest potential for off-target drift of any of the common techniques. Off-site drift is a process of key interest to the Agency. This discussion of the aerial spraying model is followed by a discussion of techniques to simulate ground-based spraying and user options for other types of applications.

3.1.1.1 Aerial Spraying--

Aerial spraying of pesticides, herbicides, and fungicides is commonly used to control insects, weeds, and plant or tree diseases in forests and crop lands. Aerial spraying models simulate the behavior of sprayed material from the time it is released from the aircraft until it has been deposited on the soil and/or vegetation. These models should also be able to simulate the concentration of the sprayed material during application; the extent of coverage and the drift beyond targeted areas; and the deposition of the material above, within, and below vegetative canopies. The processes and most significant factors which affect the fate of aerially sprayed material are discussed in the following paragraphs.

Five groups of factors can be recognized which will contribute to the transport and ultimate fate of chemicals applied aerially. These are:

1) Spray system characteristics
2) Vegetation characteristics
3) Spray depletion characteristics
4) Target characteristics
5) Meteorological factors

These factors are elaborated upon below.

Spray system characteristics--Important characteristics of the spray system include:

- Aircraft weight, speed, wing span, aspect ratio, etc.
- Application rate, swath width, release altitude
- Source dimensions, spray boom and nozzle type
- Physical and chemical properties of spray material: drop-size distribution, density, and volatility
- Emission location

Observations of aerial spraying show that the drops emitted from aircraft spray nozzles or tanks are quickly swept into the wakes of fixed wing or rotary aircraft. These drops are entrained into the aircraft-generated vortex system which, in general, sinks below the aircraft, grows in size, and decays in intensity as time elapses. The position, size, and shape of the vortex are controlled by the physical characteristics of the aircraft.

During the first minutes after the spray release, the wake vortices principally control the growth of the spray cloud. Except for the lateral translation of the vortex system by a crosswind, the vortices also control the position in space of the spray cloud.

After the first few minutes, when vortex circulations have decayed, meteorological factors in conjunction with gravitational settling govern the transport, diffusion, and deposition of the spray. If the aircraft altitude is less than about 1.5 to 2.0 wingspans above the deposition surface and the spray drops have sufficient settling velocities, the effective swath width and deposition of the spray is largely governed by the descent, growth, and subsequent decay of the vortex wake system generated by the aircraft. Thus, for aircraft spraying at higher altitudes, simple procedures appear to be sufficient in describing the vortex sink rate.

Emission rates and the location and duration of emission must obviously be considered for accurate prediction of the fate of the sprayed material.

Vegetation characteristics--The important vegetation characteristics to be considered include:

- Type of vegetation and dimensions, especially height
- Foliage density
- Spatial distribution

The presence or lack of vegetative cover is an important factor to be considered. If a vegetative canopy (i.e., forest canopy or tall vegetation) exists, its characteristics play an important role in determining the wind, thermal, and turbulence structures within the canopy and its effects on evaporation and impaction of spray on the target area.

If it is desired to determine the spatial distribution of deposited spray material within and below a canopy, methods which account for the canopy effects are needed. A canopy penetration model can be used to accomplish this. The canopy penetration model should be able to calculate the percentage of material which, after entering the top of the canopy, is retained at various levels within the canopy and on the soil surface underneath. Vegetative factors that affect the transport and deposition within and below the canopy include the spacing and type of foliage, height of canopy and coverage of the ground surface.

Spray depletion characteristics--Three factors are of major importance in determining deposition:

- Gravitational settling
- Evaporation
- Impaction

Gravitational settling acts as a depletion mechanism in drift calculations, and is the major mechanism ensuring effective canopy penetration. Spray dispersion models should account for gravitational settling in a manner that is consistent with conservation of mass and still be able to permit turbulent dispersion and partial reflection at the ground surface or canopy top of smaller drops.

Evaporation can significantly alter the airborne aerosol drop-size distribution as the spray cloud descends from the aircraft. The net effect of evaporation is to reduce the size of the drops in the cloud, thereby reducing gravitational settling velocities and deposition near the source and thus increasing downwind drift from the spray cloud.

The amount of spray reaching a given height within a canopy, following canopy penetration, depends upon drop impaction losses at higher levels within the canopy. These impaction losses depend on the drop size and the collection efficiency of the vegetation through which the drops are falling.

Target characteristics--Important target characteristics to be considered include:

- Geographic location and dimensions of spray area
- Topography and other surface features

The physical dimensions of the target, the topography and surface features in the target area are all important features that should be considered in the model formulation and in the selection of model input parameters. Other data, such as geographic location and total size of the spray block, must be known to specify spray line lengths and number of swaths required.

Meteorological factors--Important meteorological factors to be considered include:

- Vertical profiles of turbulence, wind speed and direction, temperature, and humidity
- Insolation
- Mixing depth

Deposition of sprayed material depends on the specification of meteorological conditions that exist during the spray release period (i.e., atmospheric stability). Parameters which reflect these conditions include vertical profiles of wind speed and temperature. After vortex effects have dissipated, wind speeds are required to calculate the time for drops of various sizes to reach the canopy and the flux of drops at any distance from the flight line. Wind speed profiles within the canopy may also be required to calculate the vertical trajectory of drops and the depletion by deposition and impaction within the canopy.

Temperature and relative humidity are needed if evaporation of the drops is to be considered either above or below the top of the canopy.

Estimates of vertical and lateral turbulence above the canopy are needed to calculate vertical and lateral dispersion of the spray cloud for drift calculations. In addition, knowledge of the depth of the surface mixing layer is important in estimating spray drift levels at longer distances from the flight line.

3.1.1.2 Ground-Based Spraying--

Ground-based applications of pesticides, herbicides, fumigants, and fungicides are routinely used to control weeds, insect damage to plants, and plant or tree diseases in forests and crop lands. There is a wide spectrum of application scenarios with ground-based application equipment. Typical application equipment includes disc sprayers, hydraulic sprayers, air sprayers and mist blowers, and fog applicators or aerosol generators. These application devices may be carried by hand, mounted on trucks, drawn by tractor, or incorporated in mobile units such as self-propelled sprayers. Application rates associated with spraying equipment are generally classified as high, low, or ultra-low volume.

Spraying recommendations vary with crop type, and may even vary for a particular crop. For example, on one crop, two different systems may be necessary. Disease (fungus) control might require spraying pressures of 200 to 400 psi and an application rate of 75 to 150 gallons per acre (gal acre^{-1}), and weed control may require spraying pressures of 40 to 80 psi and an application rate of 10 to 20 gal acre^{-1}. Due to such diversity, development of a universally applicable ground spray simulation model, or even a set of models, to encompass all ground spraying situations is difficult.

The five groups of factors identified and discussed in the previous section on aerial spraying also apply to ground-based spraying methods. Obviously, the major difference between the two is that aircraft wake effects are no longer of concern. Basically, only the spray system characteristics are different and are listed below as they apply to ground spraying.

Spray system characteristics--Important elements of ground spray systems include:

- Ground sprayer, speed, and other source characteristics
- Application rate, swath width, release height, and coverage

- Source dimensions, spray boom and nozzle type
- Physical and chemical properties of spray material: drop-size distribution, density, and volatility
- Emission location

3.1.2 Module Development

3.1.2.1 Background--

Previous discussions (Section 3.1.1.1 and Section 3.1.1.2) have identified processes and five major groups of factors which must be quantified in order to accurately describe the fate of sprayed material. The need to simulate these processes formed a set of criteria by which existing models were evaluated and selected. A literature review was conducted to identify both aerial spraying and ground spraying models which could be used to simulate the processes described above. The FSCBG model (Dumbauld et al. 1980) was chosen to provide the capability to simulate both aerial and ground spray operations.

The model is applicable for modeling spray emissions from fixed wing aircraft and helicopters having high forward speeds. The types of ground-spraying systems which produce spray clouds that can be potentially modeled as line sources include those methods in which the spray is delivered above or near the top of the plant canopy, if one exists, and where the spray is directed vertically, or nearly so, downward. Sprays that are directed upward or have significant velocities above the horizontal plane are less likely to be successfully modeled using the elevated line-source model.

Examples of ground-spraying equipment that can be modeled as line sources include:

- Some truck-mounted and tractor-drawn spraying systems
- Self-propelled, high-clearance sprayers
- Mobile boom sprayers

For those situations where the line-source model cannot be used, either because sufficient data are not available to adequately characterize the source or because the spraying method being modelled is not physically represented by a line source (e.g., an orchard air sprayer), simplistic ground spray models must be used. This is a result of the lack of more mechanistic models found in the literature.

Even though the version of FSCBG used has a canopy penetration model, it has not been included in this simulation package. Its drawbacks include extensive input requirements, the need to determine parameters of the plant or tree foliage (which may be known for various types of trees but are not well defined for the wide variety of vegetative canopies expected to be encountered), and the execution time required for the simulation of a large number of drops.

The canopy penetration method selected for use in TEEAM is based on theoretical and experimental work described by Uk and Courshee (1982) and Bache and Uk (1975). This method is based on an exponential decrease of the deposition density of the spray material with depth from the exposed canopy top. This simplified canopy penetration model was developed for optional use with either the aerial or ground spray models.

3.1.2.2 Description of the Spray Application/Deposition Model--
The following components make up the spray/deposition portions of TEEAM:

- An aerial spray deposition model (FSCBG)
- A ground spray model (FSCBG minus aircraft wake effects, essentially, an elevated line-source model)
- An alternative ground-based application model for cases in which the elevated line-source model is inappropriate
- A simplified canopy penetration model

The theoretical bases of these components are described in the following sections.

Aerial spray model (FSCBG)--The FSCBG model as implemented for use with the TEEAM model is described in this section. The discussions of FSCBG are taken primarily from Dumbauld et al. (1980). The major processes involved are simulation of aircraft wake effects, followed by the simulation of growth and gravitational settling of the spray cloud. The dosage and deposition calculations provided in FSCBG have been incorporated along with the drop evaporation algorithms. These are described in the following subsections.

Wake settling--The version of the FSCBG code described in this report contains a simple model. Prandtl and Tietjens (1934) express the sink rate ω(m s^{-1}) of a vortex system as

$$\omega = \frac{8g\ W_a}{\pi^3\ \rho_A\ b^2\ V_a}\ (10^{-3}) \tag{3-1}$$

where

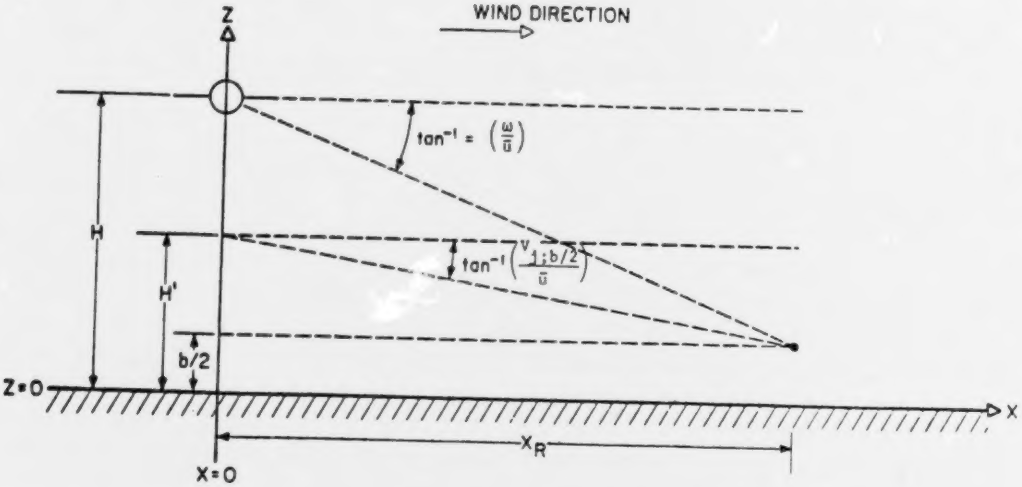
W_a = weight of the aircraft (kg)
g = acceleration due to gravity (9.8 m s^{-2})
ρ_A = air density (g cm^{-3})
b = aircraft wing span (m)
V_a = aircraft speed (m s^{-1})

Equation (3-1) is strictly applicable to fixed-wing aircraft; however, helicopter-produced vortices resemble fixed-wing vortices at high forward speeds (Dumbauld et al. 1980, p. 33) and thus Equation (3-1) is applicable to high speed helicopters.

In the spray dispersion models, the source parameters correspond to the spray cloud properties when the cloud has reached approximate atmospheric equilibrium. The vortex sink rate calculated from Equation (3-1) and the observations that the vortex tube stops descending at a distance b/2 above the ground surface (or above the canopy) are used to calculate source parameters for the models. Figure 3.1 is a schematic diagram showing the geometrical considerations used in specifying the distance downwind x_R at which cloud stabilization occurs and the effective release height H_j'. As shown in Figure 3.1, the cloud descent from the aircraft at height H forms the angle $\tan^{-1}(\omega/\bar{u})$ with the horizontal when the gravitational settling velocity for the j^{th} drop-size category at height $H(V_{j;H})$ is less than ω. In general, the FSCBG program calculates the distance downwind from the flight path where the cloud reaches a height b/2 above the surface from the expression

$$x_R = \bar{u}t_j' \qquad (3\text{-}2)$$

where


Z
WIND DIRECTION
$\tan^{-1} = \left(\frac{\omega}{\bar{u}}\right)$
H
H'
$\tan^{-1}\left(\frac{V_{j;b/2}}{\bar{u}}\right)$
b/2
Z=0
X
X_R
X=0

Source: Dumbauld, Rafferty and Bjorklund, 1977

Figure 3.1. Schematic diagram showing geometry used in constructing the distance x_r and effective source height H' for the case when the settling velocity in the j^{th} size category at height $H(V_j;H)$ is less than ω.

t'_j = effective time for the cloud centroid to reach the height b/2

$$= \begin{cases} [H - (b/2) - H_c]/\omega \; ; \; \omega \geq V_{j;H} \\ t_{j;b/2} \; ; \; \omega \leq V_{j;H} \end{cases} \qquad (3\text{-}3)$$

$V_{j;H}$ = gravitational settling velocity for the j^{th} drop-size category at the aircraft flight altitude

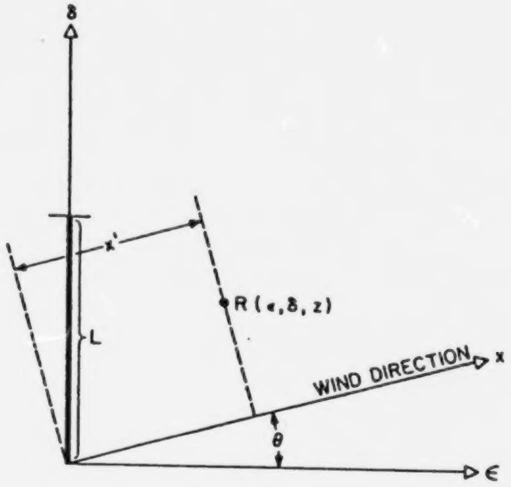
$t_{j;b/2}$ = time for the drop in the j^{th} category to reach the height $b/_2$ above the ground or canopy, calculated from the evaporation model

As discussed in more detail in the description of the spray dispersion models, the dispersion models are formulated under the assumption that the cloud axis descends at an angle $\tan^{-1} (V_j/\bar{u})$ with the horizontal. It is therefore assumed that the effective declination of the cloud axis downwind from an effective source height H'_j is given by the angle $\tan^{-1} (V_{j;b/2}/\bar{u})$, where $V_{j;b/2}$ is the gravitational settling velocity calculated by the program for the drop at the height b/2. Based on this assumption, the effective release height H'_j is

$$H'_j = H_c + (b/2) + t'_j \, V_{j;b/2} \qquad (3\text{-}4)$$

All gravitational settling velocities are calculated in the FSCBG program using a technique suggested by McDonald (1960). The graph given by McDonald expressing the relationship between the drag coefficient of spheres and their Reynolds number has been fitted for Reynolds numbers less than 2×10^5 and is used in the FSCBG program.

Spray dispersion models--In this section the models used in the FSCBG program to calculate dosage and deposition downwind from nearly instantaneous elevated line sources oriented at an arbitrary angle with respect to the mean wind direction are described. The axis of the spray cloud is assumed to be inclined from the horizontal plane by an angle that is proportional to $V_j/\bar{u}$, where V_j is the gravitational settling velocity for the j^{th} drop-size category and $\bar{u}$ is the mean cloud transport speed. When evaporation is negligible, this inclination angle is invariant with distance from the line source. For evaporating drops, the angle changes with distance from the source because V_j depends on the drop size. It is assumed that drops dispersed upwards by turbulence are totally reflected downwards at the top of the surface mixing layer, but the fraction of drops reflected at the ground is a variable input parameter for each j^{th} category. The models use the Cartesian coordinate system shown in Figure 3.2 for a line source of length L at a height H' and a calculation point at $R(\varepsilon, \delta, z)$.



Source: Dumbauld, Rafferty and Bjorklund, 1977

Figure 3.2. Schematic plan view showing the line source geometry with respect to a calculation point at $R(\epsilon, \delta, z)$ for a wind direction θ.

Dosage model--Here dosage is the integral of the concentration in the atmosphere within the spray cloud over time. Thus it represents a time-averaged concentration which can be used (together with inhalation rates) to model inhalation exposure to species of concern. In the current version of TEEAM, inhalation exposures during spray events are not computed. The dosage (mass x time/unit volume) above the canopy or soil surface is the sum of contributions from the drops in the dispersing cloud and from vapor produced by drop evaporation.

The dosage for the contribution from drops is given by the expression

$$
\begin{aligned}
D_L = \frac{S}{k\sigma_A' \sin\theta\, \bar{u}} & \sum_{j=1}^{J} f_j \Big\{ \sum_{i=0}^{\infty} \Big[\gamma_j^{\,i} \left(\frac{\pi}{2Y}\right)^{1/2} \Big\{\exp\left(\frac{0}{4Y}\right)^2 - P\Big\} \qquad (3\text{-}5) \\
& \Big\{\mathrm{erf}\left(Y^{1/2}\left(\frac{k}{a} + \frac{0}{2Y}\right)\right) - \mathrm{erf}\left(Y^{1/2}\left(\frac{k}{b} + \frac{0}{2Y}\right)\right)\Big\} \\
+ \gamma_j^{\,i+1} \left(\frac{\pi}{2Z}\right)^{1/2} & \Big\{\exp\Big(\frac{R^2}{4Z} - P\Big)\Big\}\Big\{\mathrm{erf}\Big(Z^{1/2}\left(\frac{k}{a} + \frac{R}{2Z}\right)\Big) - \mathrm{erf}\Big(Z^{1/2}\left(\frac{k}{b} + \frac{R}{2Z}\right)\Big)\Big\}\Big] \\
+ \sum_{i=1}^{\infty} \Big[\gamma_j^{\,i}\left(\frac{\pi}{2T}\right)^{1/2} & \Big\{\exp\Big(\frac{U^2}{4T} - P\Big)\Big\}\Big\{\mathrm{erf}\Big(T^{1/2}\left(\frac{k}{a} + \frac{u}{2T}\right)\Big) - \mathrm{erf}\Big(T^{1/2}\left(\frac{k}{a} + \frac{u}{2T}\right)\Big)\Big\} \\
+ \gamma_j^{\,i-1} \left(\frac{\pi}{2W}\right)^{1/2} & \Big\{\exp\Big(\frac{X}{4W} - P\Big)\Big\}\Big\{\mathrm{erf}\Big(W^{1/2}\left(\frac{k}{a} + \frac{X}{2W}\right)\Big) - \mathrm{erf}\Big(W^{1/2}\left(\frac{k}{b} + \frac{X}{2W}\right)\Big)\Big\}\Big]\Big\}
\end{aligned}
$$

where

$$S = Qk/2\pi L \tag{3-6}$$

$$Y = \frac{1}{k^2}\left[n - \frac{\delta}{\cos\theta}\right]^2 + [C + z]^2 \tag{3-7}$$

$$O = \frac{2^{1/2}}{\sigma_A' k}\left[\frac{k^2 V_j}{\bar{u}}(C + z) - \left(n - \frac{\delta}{\cos\theta}\right)\cot\theta\right] \tag{3-8}$$

$$P = \left[\frac{kV_j}{2^{1/2}\sigma_A'\bar{u}}\right]^2 + \left[\frac{\cot\theta}{2^{1/2}\sigma_A'}\right]^2 \tag{3-9}$$

$$Z = \frac{1}{k^2}\left[n - \frac{\delta}{\cos\theta}\right]^2 + [D + z]^2 \tag{3-10}$$

$$R = -\frac{2^{1/2}}{\sigma_A' k}\left[\frac{k^2 V_j}{\bar{u}}(D + z) + \left(n - \frac{\delta}{\cos\theta}\right)\cot\theta\right] \tag{3-11}$$

$$T = \frac{1}{k^2}\left[n - \frac{\delta}{\cos\theta}\right]^2 + [D - z]^2 \tag{3-12}$$

$$U = -\frac{2^{1/2}}{\sigma_A' k}\left[\frac{k^2 V_j}{\bar{u}}(D - z) + \left(n - \frac{\delta}{\cos\theta}\right)\cot\theta\right] \tag{3-13}$$

$$W = \frac{1}{k^2}\left[n - \frac{\delta}{\cos\phi}\right]^2 + [C - z]^2 \tag{3-14}$$

$$X = \frac{2^{1/2}}{\sigma_A' k}\left[\frac{k^2 V_j}{\bar{u}}(C - z) - \left(n - \frac{\delta}{\cos\theta}\right)\cot\theta\right] \tag{3-15}$$

$$C = 2iH_m - H_j' - (V_j x_V/\bar{u}) \tag{3-16}$$

$$D = 2iH_m + H_j' + (V_j x_V/\bar{u}) \tag{3-17}$$

$$a = 2^{1/2}\sigma_A' (x' + x_V - \ell \sin\theta) \tag{3-18}$$

$$b = 2^{1/2}\sigma_A' (x' + x_V) \tag{3-19}$$

$$n = (x' + x_V)\cot\theta + x'\tan\theta = (\varepsilon/\sin\theta) + (\delta/\cos\theta) + x_V\cot\theta \tag{3-20}$$

$$x' = (\varepsilon + \delta\tan\theta)\cos\theta = \varepsilon\cos\theta + \delta\sin\theta$$

x_v = virtual distance

$$= \frac{k\sigma_o}{\sigma_A'} - x_R = \frac{\sigma_o}{\sigma_E'} - x_R \qquad (3\text{-}21)$$

ℓ = effective line length

$$= \left\{ \begin{array}{ll} \delta + \varepsilon \cot\theta & ;\delta + \varepsilon \cot\theta \le L \\ L & ;\delta + \varepsilon \cot\theta > L \end{array} \right\} \qquad (3\text{-}22)$$

The following parameters used in the preceding equations are based on meteorological measurements or inferred from meteorological measurements:

σ_A' = standard deviation of the wind azimuth angle in radians

σ_E' = standard deviation of the wind elevation angle in radians

k = constant relating σ_A' and σ_E'
$= \sigma_A'/\sigma_E'$ (3-23)

H_m = depth of the surface mixing layer below a capping inversion

$\bar{u}$ = mean transport wind speed above the canopy

θ = angle between a line perpendicular to the line source and the mean wind direction (see Figure 3.2)

$\Delta\bar{u}$ = vertical wind-speed shear

The following parameters are source inputs required for use in the model:

Q = total source strength emitted along the length L of the line source

H = aircraft flight altitude above the ground

V_j = gravitational settling velocity for the median drop by mass in the j^{th} drop-size category

f_j = fraction of the total source strength in the j^{th} drop-size category

γ_j = reflection coefficient for the median drop by mass in the j^{th} drop-size category

σ_o = standard deviation of the cloud distribution at the distance x_R

L = length of the line source

As noted above, the vapor emitted from evaporating drops also contributes to the total dosage above the canopy or soil surface. In the program, the evaporation model determines the mass of vapor emitted in Δh height units along the cloud axis as it descends to the canopy. The distance downwind from the line source where the vapor is emitted is given by $\bar{u}t$, where t is the time (from the evaporation model) when the cloud axis passes through the midpoint of the height interval Δh. The source dimension of the vapor cloud emitted over the Δh height interval is

$$\sigma_o = \frac{\Delta h}{\sqrt{12}} \tag{3-24}$$

under the assumption that the vapor is rectangularly distributed at the point of emission. The vapor dosage is then calculated from Equation (3-5) with V_j set equal to zero, γ_j set to equal unity, and x_R set equal to $\bar{u}t$. Finally, the total dosage at the calculation point is determined in the program by summing the contributions from the drops and vapor clouds.

Deposition model--In TEEAM, FSCBG is used to compute the deposition of chemicals to the top of canopy or bare soil surface if no canopy exists. The deposition, expressed in units of mass per unit area, at the point (ε, δ, 0) downwind from line sources at an angle Θ with the mean wind direction is given by the expression

$$\begin{aligned}
\mathrm{Dep}_L = \frac{2S}{\sin\theta}\sum_{j=1}^{J} f_j\,(1-\gamma_j)\,\Big\{&\frac{B\exp(\frac{G^2}{4F}-P)}{2F}\Big[\exp\Big[-\big(F^{1/2}\big(\tfrac{1}{a}-\tfrac{G}{2F}\big)\big)^2\Big] \\
&-\exp\Big[-\big(F^{1/2}\big(\tfrac{1}{b}-\tfrac{G}{2F}\big)\big)^2\Big]\Big] + \frac{GB\pi^{1/2}\exp(\frac{G^2}{4F}-P)}{4F^{3/2}} \\
&\Big[\mathrm{erf}\big(F^{1/2}\big(\tfrac{1}{b}-\tfrac{G}{2F}\big)\big) - \mathrm{erf}\big(F^{1/2}\big(\tfrac{1}{a}-\tfrac{G}{2F}\big)\big)\Big] \\
&+\sum_{i=1}^{\infty}\gamma_j^{\,i-1}\,\Big\{\frac{C\exp\frac{J^2}{4I}-P}{2I}\Big[\exp\Big[-\big(I^{1/2}\big(\tfrac{1}{a}-\tfrac{J}{2I}\big)\big)^2\Big] \\
&-\exp\Big[-\big(I^{1/2}\big(\tfrac{1}{b}-\tfrac{J}{2I}\big)\big)^2\Big]\Big] + \frac{JC\pi^{1/2}\exp(\frac{J^2}{4I}-P)}{4I^{3/2}} \\
&\Big[\mathrm{erf}\big(I^{1/2}\big(\tfrac{1}{b}-\tfrac{J}{2I}\big)\big) - \mathrm{erf}\big(I^{1/2}\big(\tfrac{1}{a}-\tfrac{J}{2I}\big)\big)\Big]
\end{aligned} \tag{3-25}$$

$$+ \gamma_j \frac{D \exp\left(\frac{K^2}{4E} - P\right)}{2E} \left[\exp\left[-\left(E^{1/2}\left(\frac{1}{a} - \frac{K}{2E}\right)\right)^2\right] - \exp\left[-\left(E^{1/2}\left(\frac{1}{b} - \frac{K}{2E}\right)\right)^2\right]\right]$$

$$+ \gamma_j \frac{K D \pi^{1/2} \exp\left(\frac{K^2}{4E} - P\right)}{4E^{3/2}} \left[\mathrm{erf}\left(E^{1/2}\left(\frac{1}{b} - \frac{K}{2E}\right)\right) - \mathrm{erf}\left(E^{1/2}\left(\frac{1}{a} - \frac{K}{2E}\right)\right)\right]\Big]\Big\}\Big\}$$

$$B = H' + \frac{V_j X_v}{\bar{u}} \tag{3-26}$$

$$G = \frac{2^{1/2}}{\sigma'_A} \left[\frac{V_j B k^2}{\bar{u}} + \left(n - \frac{\delta}{\cos\theta}\right) \cot\theta\right] \tag{3-27}$$

$$F = k^2 B^2 + \left(n - \frac{\delta}{\cos\theta}\right)^2 \tag{3-28}$$

$$J = \frac{-2^{1/2}}{\sigma'_A} \left[\frac{V_j C k^2}{\bar{u}} + \left(n - \frac{\delta}{\cos\theta}\right) \cot\theta\right] \tag{3-29}$$

$$I = k^2 C^2 + \left(n - \frac{\delta}{\cos\theta}\right)^2 \tag{3-30}$$

$$K = \frac{2^{1/2}}{\sigma'_A} \left[\frac{V_j D k^2}{\bar{u}} + \left(n - \frac{\delta}{\cos\theta}\right) \cot\theta\right] \tag{3-31}$$

$$E = k^2 d^2 + \left(n - \frac{\delta}{\cos\theta}\right)^2 \tag{3-32}$$

and the remaining parameters, except a and b, are identical to those defined for the dosage model. The definitions of a and b for the dosage model given by Equations (3-18) and (3-19) are reversed in the case of the deposition model, i.e.,

$$a = 2^{1/2} \quad \sigma'_A(x' + x_V) \tag{3-33}$$

$$b = 2^{1/2} \quad \sigma'_A(x' + x_V - \ell\sin\theta) \tag{3-34}$$

Spray droplet evaporation--The FSCBG computer program allows the user to account for the effects of the evaporation of drops in the calculation of dosage and deposition. The first step in the calculation of evaporation effects is the specification of the time-rate change of the drop diameter for the initial j drop-size categories. The program user has the option of selecting an automated procedure for the theoretical calculation of the time-rate change in drop diameter (D_j), or of supplying values of the constants A, B, and C in the quadratic equation

$$D_j = A_j + B_j t + C_j t^2 \tag{3-35}$$

specifying the change of drop diameter with time t after release. The theoretical calculation of the time-rate change of drop diameter in the FSCBG program is based on the expression

$$D_{f,j} = D_{i,j} + \frac{dD}{dt} \Delta t \tag{3-36}$$

where

$D_{f,j}$ = final diameter of the median drop in the j^{th} drop-size category after the time increment Δt

$D_{i,j}$ = initial diameter of the median drop in the j^{th} drop-size category

Frössling (see Fuchs 1959, p. 44) defines the change in diameter of water drops due to evaporation by

$$\frac{dD_j}{dt} = \frac{(4 \times 10^8)\, M_\ell\, D_v\, \rho_A (e_s - e_\infty)}{M_m\, D_j\, \rho_\ell\, (P_A - e_s)}\, \bar{f}_v \tag{3-37}$$

where

M_ℓ = molecular weight of evaporating vapor from the drop (g mol^{-1})

M_m = mean molecular weight of the resulting vapor-air mixture in the transfer path which is approximated by that of air (M_A) in the FSCBG program (g mol^{-1})

D_v = molecular diffusivity of the evaporating vapor in air at the drop temperature (cm^2 s^{-1})

D_j = drop diameter (μm)

ρ_A = air density (g cm^{-3})

ρ_ℓ = density of the liquid drop (g cm^{-3})

e_s = partial pressure of the evaporating vapor at the drop surface (mb)

e_∞ = partial pressure of the evaporating vapor at an infinite distance from the drop (mb)

P_A = air pressure (mb)

$\bar{f}_v$ = ventilation factor (dimensionless)

The air density in the model is calculated from the relationship

$$\rho_a = \frac{P_A M_A}{R^* T_V} (10^{-4}) \tag{3-38}$$

where R^* is the universal gas constant (8.31432 j mole^{-1} $^oK^{-1}$) and T_V is given in terms of the mixing ratio r_∞. According to Beard and Pruppacher (1971),

$$T_V = T_A\left(1 + \frac{r_\infty}{0.62197}\right)/(1 + r_\infty) \qquad (3\text{-}39)$$

where

T_A = air temperature (^oK)

$r_\infty = 0.62197\ e_\infty/(P_A - e_\infty)$ (3-40)

The diffusivity D_v of the vapor into air at the temperature of the surface of the drop T_r depends on the liquid being considered. For water drops, the FSCBG program uses the expression (Pruppacher and Rasmussen 1979)

$$D_v = 0.211 \left[\frac{T_r}{T_o}\right]^{1.94} \left[\frac{P_o}{P_A}\right] \qquad (3\text{-}41)$$

where T_o is 273.16 ^oK, P_o is 1013.25 mb, and T_r is determined from the relation

$$T_r = T_A - \frac{L\ D_v\ M_\ell\ (e_s - e_\infty)}{k\ R^*\ T_f} \qquad (3\text{-}42)$$

where

L = latent heat of vaporization (cal g^{-1})

$= 597.3 \left[\frac{T_o}{T_r}\right]^{\alpha}$ (3-43)

$\alpha = 0.107 + 3.67 \times 10^{-4}\ T_r$ (3-44)

k = thermal conductivity (cal cm^{-1} s^{-1} $^oK^{-1}$) (3-45)

$= k_d[1 - (1.17 - 1.02\ k_v/k_d)(e_\infty/P_A)]$

$k_d = 10^{-5}[5.69 - 0.017\ (T_r - T_o)]$ (3-46)

$k_v = 10^{-5}[3.78 - 0.020\ (T_r - T_o)]$ (3-47)

$T_f = (T_r + T_A)/2$ (3-48)

The partial pressure e_s is defined by the expression

$$e_s = \beta\left[\frac{575.0466 + 31.82291\ T_i + 1.296028\ T_i^2}{93.51611 - T_i}\right] \qquad (3\text{-}49)$$

where

$T_i = T_r - T_o$ (3-50)

and

$\beta = 1$ (3-51)

The vapor pressure at e_∞ is also obtained from Equation (3-49) when T_r is replaced by T_A in Equation (3-50) and β is replaced by (RH/100), where RH is the relative humidity in percent. To find the drop temperature, vapor pressure at the drop surface, and diffusivity, Equations (3-41) through (3-49) are solved by iteration in the FSCBG program.

The ventilation factor $\overline{f}_v$ for water (Pruppacher and Rasmussen 1979) is given by

$$\overline{f}_v = \begin{cases} 0.78 + 0.308\ Sc^{1/3}\ Re^{1/2} & 1.4 < Sc^{1/3}\ Re^{1/2} \le 51.4 \\ 1.00 + 1.108\ Sc^{1/3}\ Re^{1/2} & 0 \le Sc^{1/3}\ Re^{1/2} \le 1.4 \end{cases} \qquad (3\text{-}52)$$

where

Re = Reynolds number

$$= \frac{V_j\ D_j\ \rho_A}{\mu_A}\ (10^{-4}) \qquad (3\text{-}53)$$

Sc = Schmidt number

$$= \frac{\mu_A}{D_v\ \rho_A} \qquad (3\text{-}54)$$

μ_A = absolute viscosity of air (g cm^{-1} s^{-1})

$$= \frac{(7.6342 \times 10^{-2})}{(T_A + 296.16)} \left(\frac{T_A}{296.16}\right)^{3/2} \qquad (3\text{-}55)$$

The time-rate change of drop diameter for non-water drops can also be calculated. In this case, temperature and vapor pressure of the drop are automatically calculated from the expression (Picot 1979)

$$A \exp\,(B - C/T_r) - e_s = \left(\frac{k}{C_f D_v L}\right) (T_A - T_r) \qquad (3\text{-}56)$$
$$[P_A - A \exp\,(B - C/T_t)]$$

where

A = $P_o/760$

C_f = molal concentration of the liquid (mol cm^{-3})

k = thermal conductivity of the gas mixture surrounding the drops at the drop surface temperature

B,C = constants obtained from tables expressing variations of vapor pressure with temperature (see, for example, page D-140, Handbook of Chemistry, 58th Edition, published by Chemical Rubber Co.)

Values of k, D_v, and L for non-water drops must also be specified. The value of e_∞ for non-water drops can probably be set equal to zero. When the parameters required by Equation (3-56) have been specified, the program uses Newton's iteration procedures to determine the drop temperature and vapor pressure and the time-rate change of diameter, using the following expression (Fuchs 1959) for the ventilation coefficient:

$$\bar{f}_v = \frac{1}{2} Sh \qquad (3\text{-}57)$$

where

Sh = Sherwood number

$$= 2(1 + \alpha\, Sc^{1/3}\, Re^{1/2}) \qquad (3\text{-}58)$$

and α is set equal to 0.3 in the FSCBG program as suggested by Picot (1979).

Finally, for both water and non-water drops, the results obtained using the evaporation model for above-canopy calculations are fitted with Equation (3-35) by least squares over the time period required for the drop to evaporate to a diameter of 5 micrometers or the settling velocity to reach 0.02 ms^{-1}, whichever is greater.

Alternative pesticide application methods--As previously mentioned, options are available for simulating ground based pesticide applications. These options would be used to simulate spraying events where conditions invalidate the use of FSCBG, granular applications and/or soil incorporation methods. The first involves a partitioning of deposited material between plants and soil using an exponential model. The second involves the user specification of deposition rates to foliage and soil. Even though these algorithms are in reality a part of the terrestrial fate and transport module (TFAT) they are presented here for clarity of organization.

Exponential method--This method distributes the pesticide between the plant canopy and the soil surface based on the extent of areal vegetative coverage. The fraction of applied pesticide intercepted by the foliage is given by:

$$C_F = (1 - e^{-\mu W})\, R \qquad (3\text{-}59)$$

where μ is the canopy interception coefficient ($m^2\ kg^{-1}$) W is the current value of the above ground biomass ($kg\ m^{-2}$) and R is the application rate in grams of active ingredient per square centimeter (g of cm^{-2}). C_F is not a concentration on the leaf surface, but the deposition based on projected surface area. The user may also specify the depth of penetration of the soil applied chemical so that soil incorporation techniques can be simulated.

Similarly, the fraction of applied pesticide intercepted by the soil surface is given by:

$$S_F = Re^{-\mu W} \tag{3-60}$$

where S_F is the concentration on soil surfaces not covered by the foliage.

This method does not account for any off-site drift or losses due to evaporation. Thus, all of the pesticide mass that is applied is deposited on either the plant or soil surfaces.

User-specified distribution--This method distributes the applied pesticide to the vegetative canopy and soil surface, based upon user supplied percentages for each. The equations used are:

$$C_F = P_F R \tag{3-61}$$

$$S_F = P_S R \tag{3-62}$$

where C_F and S_F (both in g cm^{-2}) are the quantities of the applied pesticide apportioned to the foliage and soil surface, respectively, P_F and P_S are the specified fractions of material allocated to the foliage and soil and R is the application rate in g of cm^{-2}. The user may also specify the depth of penetration of the soil applied chemical so that soil incorporation techniques can be simulated. Once the application rate to foliage C_F is known, this quantity can be distributed into the canopy using one of the following techniques.

Simplified canopy penetration model--The simplified canopy penetration model can optionally be used in conjunction with either the aerial (FSCBG) or ground application submodels. This model allows the user either to input the percent of spray material retained on the canopy at different levels and on the under-canopy soil or it will compute the vertical profile of deposited spray material on the vegetive canopy. The exponential decay]ethod is described in the following paragraphs followed by a brief discussion of the user specified method.

Exponential decay canopy penetration method--The exponential decay method is based on work by Uk and Courshee (1982) and Bache and Uk (1975). The model describes an exponential decrease of the deposition density of the spray with depth from the exposed canopy top, modified to account for conservation of the sprayed material.

If the entire vegetative canopy is represented by a series of discrete canopy levels, the total deposition of the spray material on a given level is described by:

$$D_i = D_o P_i \tag{3-63}$$

$$P_i = \int_o^{h_i} e^{-\beta h}\, dh - \int_o^{h_{i-1}} e^{-\beta h} dh \tag{3-64}$$

where

D_i = deposition of material in canopy level i (g cm^{-2})
h_i = distance downward from the top of the canopy to the bottom of canopy level i (cm)
D_o = initial deposition of material at the top of the canopy (g cm^{-2})
P_i = percent of material deposited in the interval h_i to h_{i-1} (canopy interval i)
β = attenuation coefficient (cm^{-1})

The total amount of material deposited on the plant canopy is given by

$$D_T = \sum_{i=1}^{n} D_i \tag{3-65}$$

where

D_T = total deposited material on canopy (g cm^{-2})
n = number of canopy levels

The remaining spray material that is not intercepted by the plant canopy is deposited on the under-canopy soil, D_s, given by:

$$D_s = D_o - D_T \tag{3-66}$$

The only external parameter which the user needs to supply is the attenuation coefficient, β. This parameter depends on the foliage density (foliage area per unit volume), impaction efficiency, and the leaf area index.

Discrete distribution canopy penetration method--This method allows the user to specify the percent of material that will be distributed to each canopy level, including the under-canopy soil surface. The submodel then calculates the deposition density based on the top-of-canopy quantity (computed by the aerial spray or ground spray models) and the percentage retained at each level.

Situations where the use of the discrete distribution canopy penetration method would be appropriate are:

- If the linear method is being used to model a sparse vegetative canopy, none of the pesticide would be deposited in the soil below the canopy, which could realistically occur. But if the discrete distribution canopy penetration method is used, the pesticide applied to the plant can be redistributed so that a specified fraction reaches the under-canopy soil.

- When an orchard, or other crop, is being sprayed from below canopy-top level, the exponential decay canopy penetration method cannot be used. If the approximate vertical distribution can be quantified, the discrete distribution canopy penetration method can be used.

3.2 TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT)

This section describes the dynamic terrestrial fate and transport module (TFAT) which is used to simulate the vertical movement of pesticides in terrestrial compartments. These compartments are made up of the soil, including the solid soil particles, the soil-air, and the soil-water, and air overlying the soil column. It is required to have the capability to simulate each of the significant chemical transport components and ancillary processes identified in Section 2. An existing transport code was selected and enhanced to serve this purpose, as described in below.

The terrestrial fate and transport module was developed in two steps. First, PRZM (Pesticide Root Zone Model, Carsel et al. 1984) was selected as the basic model. Dean et al. (1984) reviewed six pesticide fate and transport models for applicability to a similar exposure assessment problem. They selected PRZM for that application primarily because it used acceptable theory and readily obtainable input, and had good documentation. PRZM was similarly selected for inclusion in TEEAM and modifications and enhancements were added to enable it to produce the pesticide concentrations required for assessment of wildlife exposure in terrestrial ecosystems and to link it with the other TEEAM modules. The most important additions to the basic model include two groups of subroutines which simulate vapor phase transport and chemical volatilization from the soil surface and enhance the surface water hydraulics to simulate surface water ponding.

3.2.1 The Basic Fate and Transport Model (PRZM)

The Pesticide Root Zone Model is a comprehensive, dynamic, compartmental model for use in simulating chemical movement in the unsaturated soil systems within and immediately below the plant root zone. The model components are depicted in Figure 3.3.

PRZM has two major components: hydrology and chemical transport, which simulate runoff, erosion, plant uptake, leaching, decay, and foliar washoff

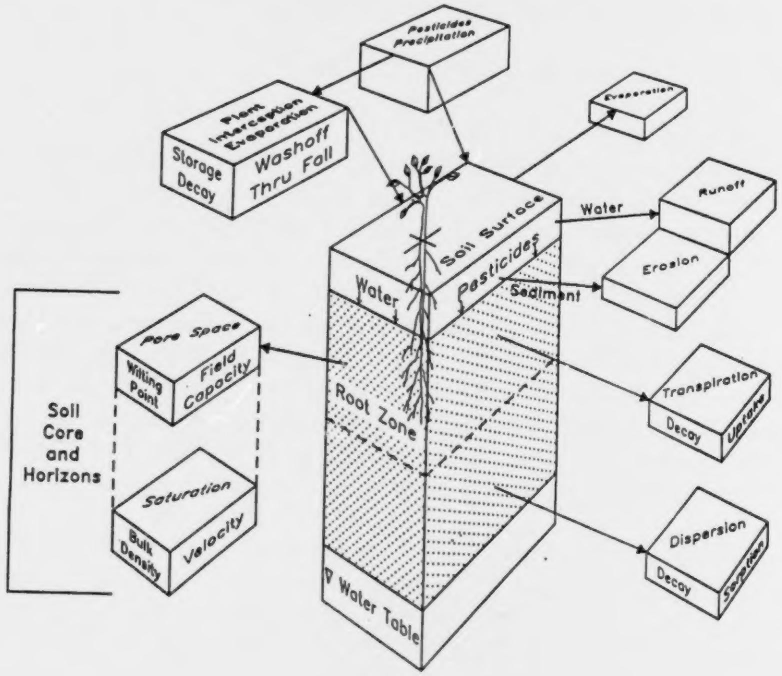

Pesticides Precipitation
Plant Interception Evaporation
Storage
Decay
Washoff
Thru Fall
Evaporation
Water
Runoff
Soil Surface
Pesticides
Erosion
Water
Sediment
Pore Space
Wilting Point
Field Capacity
Soil Core and Horizons
Root Zone
Transpiration
Decay
Uptake
Saturation
Bulk Density
Velocity
Dispersion
Decay
Sorption
Water Table

Figure 3.3 PRZM, Release 1, model components.

of a pesticide after application to an agricultural field. The hydrologic component for calculating runoff and erosion is based on the Soil Conservation Service curve number technique and the Universal Soil Loss Equation. Evapotranspiration is estimated from pan evaporation data or by an empirical formula if input pan data are unavailable. It is divided among evaporation from crop interception, evaporation from soil and ponded water, and transpiration by the crop. Water percolation is simulated by the use of generalized soil parameters including field capacity, wilting point, and saturation water content. Time-varying transport by both advection and dispersion are represented in the program. However, transport in only dissolved phases is simulated in the original program. Dissolved and adsorbed concentrations in the soil are estimated by simultaneously considering the processes of pesticide uptake by plants, surface runoff, erosion, decay, advection, foliar loss, dispersion, and retardation. The transport equations are solved utilizing a backwards-difference implicit finite-difference numerical approximation.

3.2.2 Enhancements to PRZM

The basic PRZM model was enhanced to more adequately simulate chemical fate and transport processes required for exposure assessment in terrestrial ecosystems. This required the addition of two processes which are used to simulate:

- Time-dependent infiltration and ponding

- Volatilization and vapor phase transport

Time-Dependent Infiltration and Ponding--

Soil surface hydraulics in PRZM are simple, and the enhancement of these surface water processes for the TFAT model allow for a more realistic simulation of surface water behavior and soil moisture distribution in the underlying soil during a precipitation event. In the previous releases of the PRZM model, incoming precipitation was partitioned into runoff and infiltration using the SCS curve number procedure. However, no distinction was made between water which immediately infiltrated into the subsurface and that which initially ponded on the surface and then infiltrated after some period of time. In the TFAT model, the distinction between water which infiltrates immediately and that which ponds is made, and the evolution and dissipation of the surface ponds is simulated through time.

In order to estimate chemical exposure from surface ponds, TFAT estimates the depth of the pond at a given time, the length of time for which water is ponded, and the concentration of pesticide in the ponded water. These parameters are a function of meteorological variables--especially precipitation and temperature; soil variables--soil moisture, texture, permeability, etc.; and pesticide chemistry and application history. Most of these variables are input data for other subroutines in PRZM. For example, precipitation and the soil hydraulic properties are required for the redistribution of moisture within the soil profile. The algorithm to simulate ponding was selected to impose minimal additional requirements data and utilize existing inputs to the extent possible.

One major deficiency in the structure of PRZM for the simulation of ponded water is the time step. PRZM, and the other TEEAM modules, operate on a 24-hour time step, which is too large to capture the dynamic, ephemeral nature of surface ponds. Using a finer time step in the ponding algorithm requires that each of the other hydrologic variables--precipitation, runoff, snowmelt, evapotranspiration--be disaggregated to the smaller time step and that results be reaggregated for linkage with the rest of the TEEAM model.

Volatilization--

Potential volatility of a chemical is related to its inherent vapor pressure, but actual vaporization rates depend on environmental conditions and all other factors that control behavior of the chemical at the soil/air/water interface. Several factors control volatilization from the soil surface, including pesticide properties, adsorption characteristics of the soil, pesticide concentration, soil water content, and soil temperature. Sealing of the soil surface by ponding effectively eliminates volatilization. As with the ponding algorithm, the volatilization algorithm was designed to use a minimum of new input data and merge easily with the existing transport equations.

3.2.3 Mathematical Description of the Terrestrial Fate and Transport Processes

The mathematical description of the processes simulated by TFAT are broken down in the following discussion into five categories:

- Transport in Soil
- Water Movement
- Soil Erosion
- Surface Water Ponding
- Volatilization

The first three categories were simulation options previously available in PRZM Release 1. Since the capability to simulate ponding is new, the mathematical basis of the ponding algorithm is described in detail. The final process, volatilization, was not available in previous releases of PRZM, and its theoretical basis is also described in detail.

Transport in Soil--

The pesticide transport equations in soils were derived from the conceptual, compartmentalized representation of the soil profile shown in Figure 3.4. From consideration of Figure 3.4, it is possible to write mass balance equations for both the surface zone and the subsurface zones. Addition of the vapor phase and ponded water compartments in TFAT require the consideration of additional terms. The surface zone expressions for each of the dissolved, adsorbed, and vapor phases can be written as:

$$\frac{A\Delta X\ \partial(C_w\theta)}{\partial t} = J_D - J_V - J_{DW} - J_U - J_{QR} + J_{APP} + J_{FOF} \tag{3-67}$$

$$\frac{A\Delta X\ \partial(C_s\rho_s)}{\partial t} = -J_{DS} - J_{ER} \tag{3-68}$$

$$\frac{A\Delta X\ \partial(C_g a)}{\partial t} = J_{GD} - J_{DG} \tag{3-69}$$

where

A = cross-sectional area of soil column (cm^2)
ΔX = depth dimension of compartment (cm)
C_w = dissolved concentration of pesticide (g cm^{-3})
C_s = sorbed concentration of pesticide (g g^{-1})

C_g = gaseous concentration of pesticide (g cm^{-3})
θ = volumetric water content of soil (cm^3 cm^{-3})
a = volumetric air content of the soil (cm^3 cm^{-3})
ρ_s = soil bulk density (g cm^{-3})
t = time (d)
J_D = rate of mass loss due to dispersion and diffusion of dissolved phase (g day^{-1})
J_V = rate of mass loss due to advection of dissolved phase (g day^{-1})
J_{GD} = rate of mass loss due to dispersion and diffusion in vapor phase (g day^{-1})
J_{DW} = rate of mass loss due to degradation in the dissolved phase (g day^{-1})
J_{DG} = rate of mass loss due to degradation in the vapor phase (g day^{-1})
J_U = rate of mass loss by plant uptake of dissolved phase (g day^{-1})
J_{QR} = rate of mass loss by removal in runoff (g day^{-1})
J_{APP} = mass gain due to pesticide deposition on the soil surface, including infiltration from surface ponds (g day^{-1})
J_{FOF} = mass gain due to washoff from plants to soil (g day^{-1})
J_{DS} = rate of mass loss due to degradation of sorbed phase chemical (g day^{-1})
J_{ER} = rate of mass loss by removal on eroded sediments (g day^{-1})

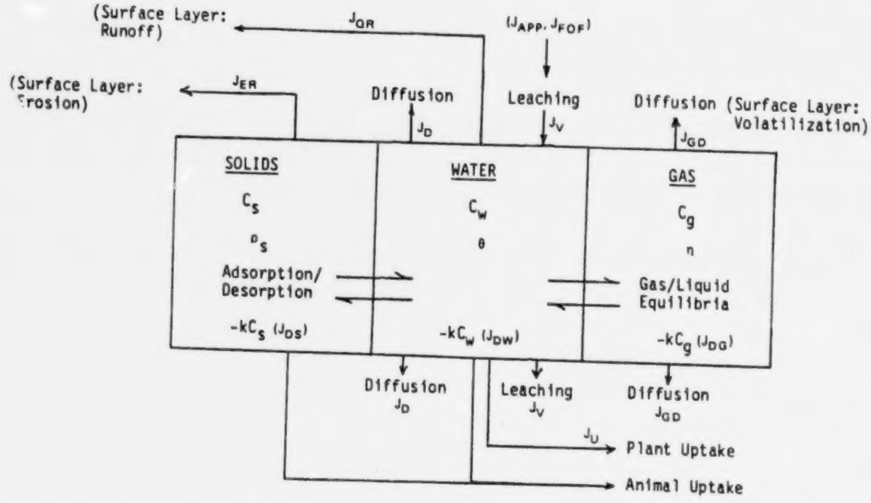
Equations for the subsurface zones are identical to Equations (3-67), (3-68), and (3-69) except that J_{QR}, J_{FOF}, and J_{ER} are not included. J_{APP} applies to subsurface zones only when pesticides are incorporated into the soil. For subsurface layers below the root zone, the term J_U is also not utilized.

Each term in Equations (3-67) through (3-69) are now further defined. Dispersion and diffusion in the dissolved phase are combined and are described using Fick's law as

$$J_D = - \frac{A\Delta X\ D_w\ \partial^2 C_w \theta}{\partial x^2} \qquad (3\text{-}70)$$

where

D_w = diffusion-plus dispersion coefficient for the dissolved phase, assumed constant (cm^2 day^{-1})
C_w = dissolved concentration of pesticide (g cm^{-3})
θ = volumetric soil water content (cm^3 cm^{-3})
x = soil depth dimension (cm)


(Surface Layer: Runoff)
J_{OR}
(J_{APP}, J_{FOF})
(Surface Layer: Erosion)
J_{ER}
Diffusion
J_D
Leaching
J_V
Diffusion (Surface Layer: Volatilization)
J_{GD}
SOLIDS
C_s
ρ_s
Adsorption/ Desorption
$-kC_s$ (J_{DS})
WATER
C_w
θ
$-kC_w$ (J_{DW})
GAS
C_g
n
Gas/Liquid Equilibria
$-kC_g$ (J_{DG})
Diffusion
J_D
Leaching
J_V
Diffusion
J_{GD}
J_U
Plant Uptake
Animal Uptake

$$C_T = C_s\rho_s + C_w\theta + C_g n$$

$$C_s = K_d C_w$$

$$C_g = K_H C_w$$

Figure 3.4 Schematic representation of a TFAT module soil layer.

In a similar manner, dispersion and diffusion in the vapor phase are described by Fick's law as

$$J_{GD} = - \frac{A\Delta X\ D_g\ \partial^2\ (C_g a)}{\partial x^2} \tag{3-71}$$

where

D_g = Molecular diffusivity of the pesticide in the air filled pore space ($cm^2\ day^{-1}$)
C_g = vapor-phase concentration of pesticide ($g\ cm^{-3}$)
a = volumetric air content ($cm^3\ cm^{-3}$)

The dependence of the molecular diffusivity of the pesticide in air filled pore space on the volumetric air content is described by the Millington-Quirk expression (Jury et al. 1983a)

$$D_g = (a^{10/3}/n^2)\ D_a \tag{3-72}$$

where

a = the air-filled porosity ($cm^3\ cm^{-3}$)
n = total porosity ($cm^3\ cm^{-3}$)

D_a = molecular diffusivity of the chemical in air, assumed constant (cm^2 day^{-1})

The mathematical theory underlying the diffusive and dispersive flux of pesticide in the vapor phase within the soil and into the overlying air can be found in the section describing volatilization.

The advective term for the dissolved phase, J_V, describes the movement of pesticide in the bulk flow field and is written as

$$J_V = \frac{A \Delta X \, V \, \partial(C_w \theta)}{\partial x} \qquad (3\text{-}73)$$

where

V = velocity of water movement (cm day^{-1})

Vapor-phase advection has not been included as a flux in the transport equation.

Degradation of a pesticide in or on soil may be due to such processes as hydrolysis, photolysis and microbial decay. If these processes follow pseudo first-order kinetics, the rate coefficients may be combined into a single decay coefficient. Assuming the same rate constants for the solid, gaseous and dissolved phases, the rate of change of chemical out of each phase due to decomposition may be written as:

$$J_{DW} = K_s C_w \theta \, A \Delta X \qquad (3\text{-}74)$$

$$J_{DS} = K_s C_s \rho_s \, A \Delta X \qquad (3\text{-}75)$$

$$J_{DG} = K_s C_g \, a \, A \Delta X \qquad (3\text{-}76)$$

where

K_s = lumped, first-order decay constant for solid and dissolved phases (day^{-1})

Plant uptake of pesticides is modeled by assuming that uptake of a pesticide by a plant is directly related to transpiration rate. The uptake is given by:

$$J_U = f \, C_w \, \theta \, \varepsilon \, A \Delta X \qquad (3\text{-}77)$$

where

J_u = uptake rate of pesticide (g day^{-1})

f = the fraction of total water in the zone used for transpiration (day^{-1})

ϵ = an uptake efficiency factor or reflectance coefficient (dimensionless)

Erosion and runoff losses as well as inputs to the surface zone from foliar washoff are considered at the soil surface. The loss of pesticide due to runoff is

$$J_{QR} = \frac{Q}{A_w} C_w A \tag{3-78}$$

in which

J_{QR} = pesticide loss due to runoff ($g\ day^{-1}$)

Q = the daily runoff ($cm^3\ day^{-1}$)

A_w = watershed area (cm^2)

and the loss of pesticide from the entire modeled area due to erosion is

$$J_{ER} = \frac{p\ X_e\ r_{om}\ C_s\ A}{A_w} \tag{3-79}$$

in which

J_{ER} = the pesticide loss due to erosion ($g\ day^{-1}$)

X_e = the erosion sediment loss ($tons\ day^{-1}$)

r_{om} = the enrichment ratio for organic matter ($g\ g^{-1}$)

p = a units conversion factor ($g\ tons^{-1}$)

Pesticides can be applied to either bare soil if pre-plant conditions prevail or to a full or developing crop canopy if post-plant treatments are desired. The pesticide application is an input mass rate which is calculated by one of the application/deposition models discussed in Section 3.1 or input directly by the user. It is partitioned between the plant canopy and the soil surface, and the rate at which it reaches the soil surface is designated J_{APP}.

Pesticides applied to the plant canopy can be transported to the soil surface as a result of washoff by rainfall. This term, J_{FOF}, is defined as:

$$J_{FOF} = E_x P_r\ M\ A \tag{3-80}$$

where

E_x = foliar extraction coefficient (cm^{-1}) (Smith and Carsel 1984)

P_r = daily rainfall depth ($cm\ day^{-1}$)

M = mass of the pesticide on the plant surface, projected area basis ($g\ cm^{-2}$)

The foliar pesticide mass, M, is further subject to degradation and loss through volatilization. Its rate of change is given by

$$\frac{AdM}{dt} = -K_f MA - J_{FOF} + A_F b \dot{A} \qquad (3\text{-}81)$$

where

K_f = lumped first-order foliar degradation constant (day^{-1})
A_F = application rate to the plant ($g\ ha^{-1}\ day^{-1}$)
b = a units conversion factor ($ha\ cm^{-2}$)

Adsorption and desorption in Equations (3-67) through (3-69) are treated as instantaneous, linear, and reversible processes. Using this assumption, the sorbed phase concentration can be related to the dissolved phase concentration by:

$$C_s = K_d C_w \qquad (3\text{-}82)$$

where

K_d = partition coefficient between the dissolved and solid phases ($cm^3\ g^{-1}$)

A similar expression can be developed to express the vapor phase concentration in terms of the dissolved phase concentration as follows

$$C_g = K_H C_w \qquad (3\text{-}83)$$

where

K_H = Henry's constant, i.e., distribution-coefficient between liquid phase and vapor phase ($cm^3\ cm^{-3}$)

Summing Equations (3-67), (3-68), and (3-69) and utilizing (3-82) and (3-83), the following expression results for the mass balance of pesticide in the uppermost soil layer.

$$\frac{\partial[C_w(\theta + K_d\rho_s + aK_H)]}{\partial t} = D_w \frac{\partial^2(C_w\theta)}{\partial x^2} + D_g \frac{\partial^2(C_w K_H)}{\partial x^2} - \frac{\partial C_w \theta V}{\partial x}$$
$$- C_w[K_s(\theta + K_D\rho_s) + K_g aK_H) + f\theta\varepsilon + \frac{Q}{A_w \Delta x} + \frac{pX_e r_{om} K_d}{A_w \Delta x}]$$
$$+ \frac{J_{APP}}{\Delta x A} + \frac{EP_r M}{\Delta x} \qquad (3\text{-}84)$$

Boundary and initial conditions are required to solve Equation 3-84. Initial conditions are input by the user as a total pesticide mass or concentration for each soil layer. Boundary values must be provided for the dissolved and vapor phase concentrations. The condition at the upper boundary for dissolved phase advection is a constant flux condition for each time step. If takes on a zero value if there is no mass flux during the time step and a positive value if there is a mass input from plant washoff or infiltration from surface ponds. The condition at the lower boundary for transport is a zero gradient

$$\frac{C_{i+1} - C_i}{\Delta x} = 0 \qquad (3\text{-}85)$$

where C_i and C_{i+1} are dissolved concentrations in the ith and i+1st compartments.

For the vapor phase, the condition at the lower boundary is also a zero gradient. The condition at the upper boundary is disscussed under the description of volatilization from soil and ponded water.

The system of equations are written in finite difference form, using central differences for diffusive terms and a backwards difference for the advection terms. The backwards difference formulation has the problem of producing some numerical dispersion. The equations are solved using a fully implicit scheme which is unconditionally stable. The Thomas algorithm is used to solve for end-of-timestep dissolved phase concentrations in each layer.

Water Movement--

Because velocity and water content of the soil are not generally known or measured as part of routine monitoring programs, it is necessary to develop additional equations for these variables in order to solve the transport equations. In the general case, Darcy's law can be combined with the continuity equation to yield the Richards equation (Richards 1931):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[K(\theta) \frac{\partial h}{\partial t}\right] \qquad (3\text{-}86)$$

$K(\theta)$ = hydraulic conductivity at various water contents (θ)
θ = soil water content

and

$$V = -K(\theta) \frac{\partial h}{\partial x} \qquad (3\text{-}87)$$

or, in simpler terms

$$\frac{\partial \theta}{\partial t} = - \frac{\partial V}{\partial x} \qquad (3\text{-}88)$$

where

V = soil water velocity (cm day^{-1})

Writing (3-88) in a backwards finite difference form yields

$$\Delta X \, (\Theta^{t+1} - \Theta^{t}) = (V_i - V_{i-1}) \, \Delta t \tag{3-89}$$

or

$$\Theta^{t+1} \, \Delta X = (V_i - V_{i-1}) \Delta t + \Theta^{t} \Delta x \tag{3-90}$$

In these equations, t and t + 1 denote the beginning and end of time step values, respectively, and i is the soil layer index. These equations can be further simplified by substituting the nomenclature SW for $\Theta\Delta X$ so that

$$SW^{t+1} = SW^{t} + (V_i - V_{i-1}) \, \Delta t \tag{3-91}$$

where

SW = soil water content (cm).

The velocities shown in Equation (3-91) are a function of inputs to the soil (precipitation, infiltration) and outflows from the soil (evapotranspiration, runoff).

Water balance equations are separately developed for (a) the surface zone, (b) horizons comprising the active root zones, and (c) the remaining lower horizons within the unsaturated zone. The equations are:

Surface Zone

$$(SW)_1^{t+1} = (SW)_1^{t} + INF - I_1 - E_1 - U_1 \tag{3-92}$$

Root Zone

$$(SW)_i^{t+1} = (SW)_i^{t} + I_{i-1} - U_i - I_i \tag{3-93}$$

Below Root Zone

$$(SW)_i^{t+1} = (SW)_i^{t} + I_{i-1} - I_i \tag{3-94}$$

where

$(SW)_i^t$ = soil water in layer "i" on day "t" (cm)

E_i = evaporation (cm day^{-1})
U_i = transpiration (cm day^{-1})
I_i = percolation out of zone i (cm day^{-1})
INF = infiltration into layer 1 (cm day^{-1})

Daily computation of soil moisture in the soil profile using the above equations requires the additional calculations for infiltration, evaporation, transpiration, and percolation.

Infiltration is calculated as

$$INF = P + SM - Q - \Delta DP - E - U \tag{3-95}$$

where

P = precipitation as rainfall, minus crop interception (cm day^{-1})
SM = snowmelt (cm day^{-1})
Q = runoff depth (cm day^{-1})
E = evaporation (cm day^{-1})
U = evapotranspiration (cm day^{-1})
ΔDP= increase in depth of ponded surface water (cm day^{-1})

The calculation of precipitation, snowmelt, and runoff on a daily time step as calculated in TFAT are described below. The disaggregation of these values and the calculation of the change in the depth of ponding on a finer time step is included in the section describing the simulation of ponded surface water.

Precipitation pan evaporation and/or air temperature are first read from an input file. Incoming precipitation is first partitioned between snow or rain, depending upon temperature. Air temperatures below 0.0°C produce snow and may result in the accumulation of a snowpack. Precipi-tation first encounters the plant canopy and once the interception storage is depleted, the remaining depth is available for the runoff or infiltration.

The runoff calculation partitions the precipitation between infiltrating water and surface runoff. Infiltrating water may be ponded on the soil surface for a period of time before it infiltrates (this process is described in a subsequent section). Runoff is calculated by a modification of the USDA Soil Conservation Service curve number approach (Haith and Loehr 1979). Snowmelt is estimated on days in which a snow pack exists and above freezing temperatures occur as

$$SM = C_M T \tag{3-97}$$

where

C_M = degree day snowmelt factor (cm °C^{-1} day^{-1})
T = average daily temperature (°C)

The precipitation and/or snowmelt are inputs to the SCS runoff equation used to compute runoff depth Q:

$$Q = \frac{(P + SM - 0.2S)^2}{P + SM + 0.8S} \tag{3-98}$$

where S, the watershed retention parameter, is estimated by

$$S = 1000/RCN - 10 \tag{3-99}$$

where RCN = SCS runoff curve number

Curve numbers are a function of soil type, soil drainage properties, crop type, and management practice. Typically, specific curve numbers for a given rainfall event are determined by the sum of the rainfall totals for the previous 5 days, known as the 5-day antecedent moisture condition. In TFAT, as in the original version of PRZM, the curve numbers are continuously adjusted each day as a function of the soil water content in the upper soil layers. These algorithms were developed and reported by Haith and Loehr (1979).

The daily evaporative demand is divided among evaporation from canopy, ponded surface water, soil evaporation, and crop transpiration. Total demand is first estimated and then extracted sequentially from crop canopy storage, ponded surface water, and then from each layer until wilting point is reached in each layer or until total demand is met. Evaporation occurs down to a user-specified depth. The remaining demand, crop transpiration, is met from the active root zone. The root zone growth function is activated at crop emergence and increases stepwise until maximum rooting depth is achieved at crop maturity.

Actual transpiration from a soil layer is estimated as:

$$U_i = \text{MIN}\ [(SW_i - WP_i)\ f_{di},\ ET_p - \sum_{1}^{i-1} U_i] \tag{3-100}$$

where

U_i = the actual transpiration from layer 'i' (cm)
f_{di} = depth factor for layer 'i'
WP_i = wilting point water content in layer 'i' (cm)
ET_p = potential evapotranspiration (cm)

This equation states that the transpiration from any layer 'i' is the minimum of the available water in layer 'i' or the demand remaining after extracting available water from layers above 'i' in the profile.

The depth factor, f_{di}, is internally set in the code. It linearly weights the extraction of transpired water from the root zone with depth. A triangular root distribution is assumed from the surface zone to the maximum depth of rooting with the maximum root density assumed to be near the surface. This algorithm essentially views the plant as a pump and assumes that it will expend the minimum energy possible in pumping. As long as the soil water is equally available, water closest to the surface meets this criteria.

Transpiration may also be limited by soil moisture availability. The potential rate may not be met if sufficient soil water is not available to meet the demand. In that case, TFAT modifies the potential rate by the following equations:

$$\begin{aligned} ET_p &= ET_p && \text{if } SW \geq 0.6\ FC \\ ET_p &= SMFAC\ ET_p && \text{if } WP < WS < 0.6\ FC \\ ET_p &= 0 && \text{if } SW \leq WP \end{aligned} \qquad (3\text{-}101)$$

where

FC = soil moisture content at field capacity (cm)
WP = soil moisture content at wilting point (cm)
SMFAC = soil moisture factor

The SMFAC concept has been used in other similar water balance models (Haith and Loehr 1979; Stewart et al. 1976) and is internally set in the code to linearly reduce ET_p according to the limits imposed in Equation (3-100). If pan evaporation input data are available, ET_p is related to the input values by

$$ET_p = C_p\ PE \qquad (3\text{-}102)$$

where

PE = pan evaporation (cm day^{-1})
C_p = pan factor (dimensionless)

The pan factor is constant for a given location and is a function of the average daily relative humidity, average daily wind speed, and location of the pan with respect to an actively transpiring crop.

In the absence of pan evaporation data, ET_p is estimated by

$$ET_p = 14000\ L_d^2(SVD) \qquad (3\text{-}103)$$

where

L_d = possible hours of sunshine per day, in 12-hour units
SVD = 0.622 SVP/(R_g T_{abs}) and
SVP = saturated vapor pressure at the mean absolute air temperature (mb)
R_g = dry-air gas constant
T_{abs} = absolute mean air temperature (°K)

The final term in the water balance equations that must be defined is the percolation value, I. The use of the SCS curve number approach for runoff precludes the direct use of a Darcian model. TFAT, like PRZM, resorts to "drainage rules" keyed to soil moisture storages and the time available for drainage. Two options are included. Although these options are admittedly simplistic representations of soil moisture redistribution, they are consistent with the objectives of TEEAM and its intended uses.

Option 1--Percolation, I, in this option is defined in the context of two bulk soil moisture holding characteristics commonly reported for agricultural soils: field capacity and wilting point. Field capacity is a somewhat imprecise measure of soil water holding properties and is usually reported as the moisture content that field soils attain after all excess water is drained from the system under influence of gravity, usually at tensions of about 0.3 bar. The difficulty with this concept is the fact that some soils will continue to drain for long periods of time, and thus field capacity is not a constant. Admitting the lack of theoretical and physical rigor, the concept remains as a useful measure of soil moisture capacity and has been successfully used in a number of water balance models (Haith and Loehr 1979; Stewart et al. 1976). Wilting point is a function of both the soil and plants growing in the soil. It is defined as the soil moisture content below which plants are unable to extract water, usually at tensions of about 15 bar.

Field capacity and wilting point are used operationally to define two reference states in each soil layer for predicting percolation. If the soil water, SW, is calculated to be in excess of field capacity, then percolation is allowed to remove the excess water to a lower zone. The entire soil profile excess is assumed to drain within one day. The lower limit of soil water permitted is the wilting point. One outcome of these assumed "drainage rules" is that the soil layers below the root zone tend to quickly reach field capacity and remain at that value. When this condition is reached, all water percolated below the root zone will displace the water within the lower soil layer simulated, and so on. There is no allowance for lateral water movement. Water balance accounting in this manner should be most accurate for sandy soils in which water movement is relatively unimpeded and is least accurate for clay soils (Stewart et al. 1976).

Option 2--The second option is provided to accommodate soils having low permeability layers that restrict the "free drainage" assumed in Option 1. In the context of the field capacity reference condition, two things may occur. First, conditions may prevail that raise the soil moisture levels above field capacity for periods of time because the water is "backed up" above a relatively impermeable layer. Second, the excess water may not drain during the one-day period assumed in Option 1. To accommodate these conditions, two additional parameters are needed. Maximum soil moisture storage, (or porosity) Θ_s, is added to represent moisture contents under saturated conditions. The drainage rate also must be modified to allow drainage to field capacity over periods in excess of one day (one time step). This is accomplished by adjusting the end of time step moisture content by

$$\Theta_i^{t+1} = (\Theta_i^{t*} - \Theta_{fc_i}) \exp(-\alpha \Delta t) + \Theta_{fc_i} \qquad (3\text{-}104)$$

where

Θ = soil layer water content ($cm^3\ cm^{-3}$)
Θ_{fc} = water content at field capacity ($cm^3\ cm^{-3}$)
α = drainage rate parameter (day^{-1})
i = the layer index

In this equation, t and t+1 denote beginning and end of time step values, respectively, and i is the soil layer index. The value t* denotes a value of time between beginning and end of time step. The variable Θ_i^{t*} here denotes current storage plus any percolation from the next layer above, before the occurrence of any drainage from the current layer. Because Equation (3-103) is solved independently for each layer in the profile, there is a possibility of exceeding the storage capability (saturation water content, Θ_s) of a low-permeability layer in the profile if a more permeable layer overlies it. At each time step, once redistribution is complete, the model searches the profile for any $\Theta_i > \Theta_{s_i}$. If this condition is found, the model redistributes water back into overlying layers, as if the percolation of additional water beyond that necessary to saturate the low-permeability layer had not occurred. This adjustment is necessary due to the nature of Equation (3-103) and the fact that these equations for each layer are not easily coupled. The difficulty in coupling the equations for the entire profile arises from the dichotomy that one of two factors limits percolation from a stratum in the profile: either the rate at which that stratum can transmit water, or the ability of the stratum below it to store or transmit water. This dichotomy would lead to an iterative (or at least corrective) approach to the explicit solution of a system of equations for Θ_i, represented by Equation (3-103). It should be noted, however, that the value of α selected by this approach is only relevant if the permeability of the soil materials, and not storage considerations in the profile (i.e., the presence of a water table), is the limiting factor for percolation of water.

During those time periods when precipitation is occurring or water is ponded at the surface, the hydraulic simulation in TFAT defaults to a third algorithm in preference to options 1 or 2, which normally redistribute water in the profile. The use of this third algorithm is required by the assumptions inherent in the Green-Ampt model which is utilized to simulate surface water infiltration and ponding. The model assumes a piston-like downward movement of a sharply defined wetting front, behind which the soil is completely saturated, and in front of which it remains at its initial water content. When these conditions no longer hold, the user-specified option is again used for percolation calculations.

Soil erosion--Removal of sorbed pesticides on eroded sediments requires estimates for soil erosion. The Modified Universal Soil Loss Equation (MUSLE) as developed by Williams (1975) is used to calculate soil loss

$$X_e = a\,(V_r q_p)^{0.56} K\ LS\ C\ P \tag{3-105}$$

where

X_e soil loss (tons day^{-1})
V_r = volume of event (daily) runoff (m^3)
q_p = peak storm runoff ($m^3 \sec^{-1}$)
K = soil erodability factor
LS = length-slope factor
C = soil cover factor
P = conservation practice factor
a = units conversion factor

Most of the parameters in Equation (3-104) are easily determined from other calculations within PRZM (e.g., V_r), and others are familiar terms readily available from handbooks. However, the peak storm runoff value, q_p, can vary widely. A trapezoidal hydrograph is assumed in TFAT with a stochastically determined average storm duration, as described later in this section under the discussion of surface water ponding. From the assumed hydrograph shape and the storm duration, a peak runoff rate is calculated.

The enrichment ratio, r_{om}, is the remaining term which needs to be defined to estimate the removal of sorbed pesticides by erosion. Because erosion is a selective process during runoff events, eroded sediments become "enriched" in smaller particles. The sediment transport theory available to describe this process requires substantially more hydraulic spatial and temporal resolution than used in PRZM, leading to the adoption of an empirical approach (Mockus 1972). The enrichment ratio for organic matter is calculated from

$$\ln(r_{om}) = 2 + 0.2\ \ln(X_e/A_w) \tag{3-106}$$

in which A_w is the area of the habitat.

Surface water ponding--Surface water ponding is the accumulation of excess water at the soil surface. Ponding occurs when the surface soil layers are saturated and consists of water which does not infiltrate, evaporate, or runoff. Pesticides may enter ponded water through direct application or washoff from plants; ponded water can therefore be an important route of exposure for animals which drink or bathe in ponds. Simulation of surface ponds involves modeling both the movement of water through ponds and the fate of chemicals dissolved in ponded water.

The movement of water through ponds is modeled in the TFAT module using a water balance approach to calculate changes in pond depth over time:

$$DP^t = DP^{t-1} + P^t - Q^t - E^t - I^t \tag{3-107}$$

where

DP^t = the depth of ponding at time t (cm)
P^t = the amount of precipitation occurring during a time step Δt (cm)
Q^t = the runoff during time step Δt (cm)
E^t = evaporation during time step Δt (cm)
I^t = infiltration during time step Δt (cm)

Because ponding is an ephemeral process which depends on rapidly varying rates of infiltration, runoff, and precipitation, the water balance equation is solved using time steps smaller than the daily TFAT step (i.e., hourly). Daily values of precipitation and runoff are dissaggregated into values for smaller time steps by assuming representative shapes of the rainfall hydrograph and the runoff hydrograph. Calculation of the individual components of the water balance is discussed in the following paragraphs.

The TFAT module uses daily values of precipitation depth; use of these daily depths in pond water balance calculations requires knowledge of the timing of precipitation. The duration of precipitation events is estimated using an empirical relationship:

$$T_d = a(\mathrm{PRECIP})^b \tag{3-108}$$

where

T_d = rainfall duration (hrs)
a = empirical constant ($\mathrm{hr\ cm}^{-b}$)
b = dimensionless exponent
PRECIP = the daily precipitation depth (cm)

The coefficients a and b will vary depending on the type of storms encountered in the region of interest. Although a and b will in reality also vary from storm to storm and seasonally, it is assumed that they are constants for a given location. Once the duration of the storm is estimated, the precipitation amount for ponding time steps is calculated by assuming uniform precipitation over the storm duration:

$$P^t = (\mathrm{PRECIP}/t_d)\Delta t, \quad 0 \leq t \leq T_d \tag{3-109}$$
$$= 0 \qquad\qquad t > T_d$$

where ΔT = the ponding time step (hours)

The amount of runoff occurring during ponding time steps is obtained by integrating the runoff hydrograph over each time step:

$$Q^t = \int_t^{t+\Delta t} q(t)dt \tag{3-110}$$

where $q(t)$ is the runoff rate at time t ($\mathrm{cm\ hr}^{-1}$). For TFAT runoff an SCS trapezoidal hydrograph is assumed, as defined by the peak flow rate, the storm duration, and the time of concentration for storms (see Figure 3.5). The time of concentration T_c (hours) describes the rise and fall of the hydrograph and is a user input parameter which is a function of the topography of the simulated drainage area. The peak runoff rate is calculated from the total runoff volume:

$$q_p = \frac{Q}{T_d - T_a} \tag{3-111}$$

where

q_p = the peak runoff rate ($\mathrm{cm\ hr}^{-1}$)
Q = the total runoff volume, calculated from Equation 3-98 (cm)

T_a is the time of initial abstraction, or the lag time between the start of the storm and the beginning of runoff:

$$T_a = \frac{0.2\ T_d S}{\mathrm{PRECIP}} \tag{3-112}$$

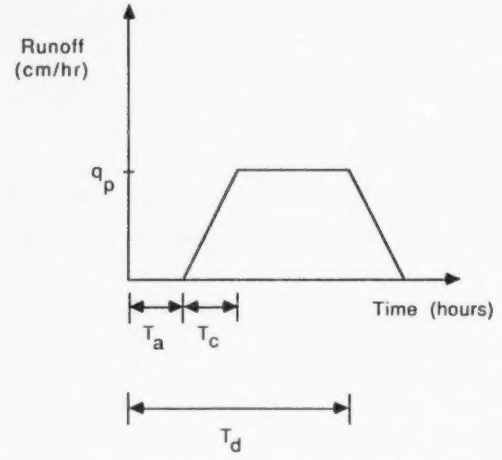


Figure 3.5 SCS trapezoidal runoff hydrograph.

S in the above equation is the SCS watershed retention parameter defined by Equation (3-99).

The infiltration capacity of the soil is estimated using the Green-Ampt equation. This infiltration model, developed by Green and Ampt (1911), relates the infiltration rate to the length of the soil wetting front. The soil is assumed to be saturated behind the front and infiltration is driven by gravity and capillary suction in the unsaturated soil ahead of the wetting front. The infiltration rate equation is then given by:

$$\frac{dF}{dt} = K_s\left[1 + \frac{(DP + H_f)a}{F}\right] \qquad (3\text{-}113)$$

where

F = the cumulative infiltration depth (cm)
K_s = the saturated hydraulic conductivity of the soil (cm/hr)
H_f = a capillary suction parameter (cm)
a = the available (i.e., air) porosity ($cm^3\ cm^{-3}$)

The soil infiltration capacity computed by the Green-Ampt model starts at an infinite rate and decreases with time to an asymptotic rate equal to K_s. The Green-Ampt rate equation cannot be analytically integrated to obtain infiltration amount unless the depth of ponding is constant. The ponding algorithm therefore assumes for each time step that the pond depth is a constant equal to the start of time step depth for infiltration calculations. The integrated Green-Ampt equation under these conditions is:

$$(F^{t+1} - F^{t}) = K_s \, \Delta t + H \ln (H + F^{t+1}) - H \ln (H + F^{t}) \qquad (3\text{-}114)$$

where

$H = (DP^{t} + H_f)n$
F^{t} = infiltration amount at the start of the time step (cm)
F^{t+1} = infiltration amount at the end of the time step (cm)

The integrated Green-Ampt equation is solved by second-order Taylor series iteration for the end of time step infiltration capacity. This infiltration depth (F^{t+1}) is the amount which can potentially occur according to soil moisture conditions. The actual infiltration depth occurring during the time step will be the minimum of the infiltration capacity and the amount of available pond water:

$$\begin{aligned} I^{t} &= F^{t+1} - F^{t} & \qquad F^{t+1} - F^{t} &\leq AW \\ &= AW & \qquad F^{t+1} - F^{t} &\geq AW \end{aligned} \qquad (3\text{-}115)$$

where

AW = available water (cm)
$= DP^{t} + P^{t} - Q^{t}$

Thus, using the precipitation amount (P^{t}) SCS runoff volume (Q^{t}) and the infiltration volume (I^{t}), the pond water balance (Equation 3-107) is solved for the depth of ponding at the end of each ponding time step within the TFAT daily step. As discussed previously, evaporation demand is met sequentially by the plant canopy, ponded water, and soil water. Therefore, evaporation calculations are decoupled from the pond water balance so that canopy evaporation can be used first to meet evaporation demand. Evaporation is then subtracted from the pond depth at the end of each TFAT daily time step. While it is recognized that this does not account for variations in evaporation during the day, evaporation losses are usually small during the precipitation events which produce ponds.

Chemical Fate and Transport in Ponded Water--

Toxic chemicals in ponded water undergo a number of transport and transformation processes. Pesticides may advect into the soil column by infiltration, volatilize through the air-water interface, and degrade through various chemical and biochemical reactions. These processes are summarized in Figure 3.6. The total change in chemical mass in ponds over time may be written in differential form as:

$$\frac{dC_pV}{dt} = -J_A - J_{pv} - J_{DC} + J_L - J_{AN} \qquad (3\text{-}116)$$

where

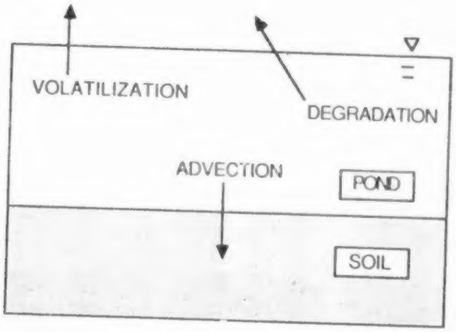
C_p = total concentration of chemical in ponded water (g cm^{-3})
V = volume of ponded water (cm^3)
J_A = mass flux of chemical due to advection resulting from infiltration (g day^{-1})
J_{pv} = mass flux of the chemical due to volatilization (g day^{-1})
J_{DC} = mass flux flux due to chemical decay (g day^{-1})
J_L = mass flux due to chemical loading (g day^{-1})
J_{AN} = mass flux due to animal utilization (g day^{-1})

Advection is simply the transport of chemical into the soil as water infiltrates into the soil. The advective flux for a well-mixed pond is given by:

$$J_A = INF\ A\ C_p \tag{3-117}$$

where

INF = pond filtration rate, computed from the Green-Ampt equation (cm day^{-1})
A = surface area of pond (cm^2)



IMPORTANT PROCESSES:

1. VOLATILIZATION OF DISSOLVED PHASE.
2. CHEMICAL AND BIOLOGICAL DEGRADATION.
3. ADVECTION INTO THE SOIL MATRIX.

Figure 3.6 Chemical transport and fate in ponded water.

Volatilization results from concentration gradients at the air-liquid interface. The pond volatilization flux is modeled as a diffusion process through boundary layers within the pond and in the overlying air. The diffusive flux through the water boundary layer is computed from the concentration gradient between the center of the pond and the pond surface:

$$J_{pv} = A\ D_w \frac{(C_p - C_{ps}/K_H)}{0.5(DP)} \tag{3-118}$$

where:

D_w = the diffusion coefficient of chemical in water ($cm^2\ day^{-1}$)
C_{ps} = the vapor phase concentration of chemical at the air-liquid interface ($g\ cm^{-3}$)
K_H = Henry's law constant for the chemical ($cm^3\ cm^{-3}$)

This equation assumes that the concentration at the center of the pond equals the average concentration, C_p. The flux through the air boundary layer is computed assuming a linear concentration gradient through the plant canopy and zero concentration at the top of the plant canopy:

$$J_{pv} = A\ D_a \frac{C_{ps}}{Z_{CH}} \tag{3-119}$$

where

D_a = the vapor-phase diffusion coefficient for the chemical $cm^2\ day^{-1}$)
Z_{CH} = the height of the plant canopy

Equating the two boundary fluxes and solving for the vapor phase concentration at the pond surface:

$$C_{ps} = \frac{2\ D_w\ C_p}{DP \frac{D_a}{Z_{CH}} + \frac{2\ D_w}{K_H}} \tag{3-120}$$

The flux out of the pond can then be computed by substituting the above expression into the air boundary layer flux equation:

$$J_{pv} = \frac{(2\ D_w\ C_p)}{(DP \frac{D_a}{Z_{CH}} + \frac{2\ D_w}{K_H})} \frac{A\ D_a}{Z_{CH}} = A\ K_v\ C_p \tag{3-121}$$

in which

K_v = a volatilization rate parameter ($cm\ day^{-1}$) which will vary with the depth of ponding

Chemical degradation in ponds may occur by hydrolysis, photolysis, biodegradation, and a number of other transformation processes. A detailed description of the chemical reactions occurring in ponded water is beyond the scope of this model. Degradation is assumed to be the same in both the dissolved and adsorbed phases and is therefore modeled by a simple first-order decay process:

$$J_{DC} = k_p C_p V \qquad (3\text{-}122)$$

where

k_p = lumped first-order decay constant (day^{-1})

Chemical fluxes due to loading and animal uptake are simulated in other TEEAM modules and subroutines. The pesticide spray and deposition model accounts for the largest portion of the pesticide load. Other loads may occur due to leaf washoff. Animal uptake losses are derived in the food chain portion of TEEAM.

The individual pond chemical fluxes due to advection, volatilization, and decay are derived as discussed above. Substituting these relationships into the pond chemical mass balance equation and dividing by the area of the pond yields the following expression:

$$\frac{d(C_p DP)}{dt} = -(INF)C_p - K_v C_p - K_p(DP)C_p - K_A C_p - L \qquad (3\text{-}123)$$

where:

K_A = first order animal uptake rate constant, computed in the APUM module (cm day^{-1})

L = total loading rate per unit area (g cm^{-2} day^{-1})

If it is assumed that the depth of ponding DP is constant over each ponding time step (the time step used in the pond water balance calculations), the mass balance equation can then be written in terms of lumped first order constants:

$$\frac{dC_p}{dt} = K_1 C_p + K_2 \qquad (3\text{-}124)$$

where:

$$K_1 = 1/DP(-INF - K_v - K_p DP - K_A) \qquad (3\text{-}125)$$
$$K_2 = L/DP \qquad (3\text{-}126)$$

The above equation is integrated and solved analytically for the pond chemical concentration at the end of each ponding time step (during which the pond depth is assumed to be equal to the start of time step depth):

$$C_p^{t+1} = e^{K_1 \Delta T}\left[C_p{}^t + \frac{K_2}{K_1}\right] - \frac{K_2}{K_1} \qquad (3\text{-}127)$$

C_p^{t+1} is the concentration at the end of the time step, and C_p^t is the concentration at the beginning of the time step. K_1 and K_2 are constants over individual time steps but are updated at the start of each time step to account for changes in pond depth and infiltrate rate computed by the pond water balance equation. Note that the time step used to solve the pond chemical mass balance equation is the same as that used for the pond water balance equation.

Volatilization from the Soil Surface--

Volatilization (i.e., vapor flux) of pesticide at the soil surface is modeled in a manner similar to that described for volatilization from ponds. The diffusive flux out of the soil is approximated using a linear concentration gradient from the center of the top soil layer to the soil surface:

$$J_{GD} = D_g A[C_{g,1} - C_{g,s}] \qquad (3\text{-}128)$$

$C_{g,1}$ = vapor-phase concentration in the surface soil layer (g cm^{-3})
$C_{g,s}$ = vapor-phase concentration at the soil-atmosphere interface (g cm^{-3})
D_g = the vapor diffusion coefficient in soil (cm^2 day^{-1}) (see Equation (3-72))

This expression assumes that the concentration at the center of the top soil layer is equal to the average concentration in the layer. The vapor phase concentration in soil is related to the dissolved phase concentration by the Henry's law equilibrium relationship (Equation (3-83)). The flux through the boundary layer of air above the soil is given by assuming a linear concentration gradient through the plant canopy and zero concentration at the top of the plant canopy:

$$J_{GD} = D_a A \frac{C_{g,s}}{Z_{CH}} \qquad (3\text{-}129)$$

Equating the two boundary fluxes and solving for the concentration at the atmosphere-soil interface:

$$C_{gs} = \frac{2\,D_g\,C_{g,1}}{\frac{D_x D_a}{Z_{CH}} + 2D_g} \qquad (3\text{-}130)$$

The vapor flux boundary condition at the soil surface can then be defined in terms of the top soil layer vapor concentration ($C_{g,1}$) by substituting the above expression into the atmospheric flux equation:

$$J_{GD} = \left(\frac{2\ D_g\ C_{g,1}}{\frac{D_x D_a}{Z_{CH}} + 2D_g}\right) \frac{D_a A}{Z_{CH}} \tag{3-131}$$

$$= \left(\frac{2\ D_g\ D_a\ A}{D_x D_a + 2\ D_g\ Z_{CH}}\right) C_{g,1}$$

Thus, the vapor flux boundary condition at the soil surface is calculated as a function of the vapor concentration in the top soil layer and the height of the plant canopy. Note that if ponds are present, there is no vapor phase at the soil surface and the volatilization flux out of the soil is zero.

Volatilization Flux through the Plant Canopy--

In pioneering work on this topic, Parmele et al. (1972) discuss a number of micrometeorological techniques for calculating pesticide volatilization flux from observed aerial pesticide concentrations. Their procedures are based on the assumption that the vertical diffusivity coefficient (K_z) for pesticide vapor is analogous to the vertical diffusivity for water vapor, energy, or momentum. The pesticide volatilization flux can be computed by Fick's first law of diffusion, as follows:

$$J_z(Z) = -\ K_z(Z)\ (dP/dZ) \tag{3-132}$$

where

$J_z(Z)$ = pesticide flux at height Z ($g\ m^{-2}\ s^{-1}$)

(dP/dZ) = pesticide concentration gradient in the canopy atmosphere ($g\ m^{-2}$)

$K_z(Z)$ = the vertical diffusivity at the height Z ($m^2\ s^{-1}$)

The value of K_z depends on the turbulent flow of the atmosphere into which the pesticide vapor is dissipated. Therefore, it is a function of the prevailing meteorological conditions and not of any physical or chemical property of the pesticide.

In order to apply these concepts, pesticide concentrations at two or more heights are required to estimate the pesticide gradient and the subsequent flux. For the estimation of vertical diffusivity, more extensive meteorological information is also required. All of these data requirements pose significant limitations for a predictive modeling approach consistent with expected and current TEEAM users.

To avoid supplying the model with such extensive meteorological data, a relationship for K_z is derived in the following paragraphs as a function of height within the canopy. Then one need only to consider the pesticide concentration gradient (or a suitable surrogate) in order to compute the pesticide volatilization flux.

Estimation of $K_z(Z)$--Mehlenbacher and Whitfield (1977) present the following formula to compute K_z at various heights within the plant canopy:

$$K_z(Z) = K_z(Z_{CH}) \exp(4.0 (\frac{Z}{Z_{CH}} - 1.0)) \tag{3-133}$$

$$K_z(Z_{CH}) = U^* \, k \, (Z_{CH} - \underline{D})/\phi h \tag{3-134}$$

$$U^* = \frac{k \, U_{CH}}{\ln((Z_{CH} - \underline{D}/Z_o) + \psi_m(\phi_m))} \tag{3-135}$$

where

$K_z(Z)$ = thermal eddy diffusivity at height Z ($m^2 \, s^{-1}$)
$K_z(Z_{CH})$ = thermal eddy diffusivity at canopy height ($m^2 \, s^{-1}$)
Z_{CH} = canopy height (m)
Z_o = roughness length (m)
$\underline{D}$ = zero plane displacement height (m)
k = von Karman's constant, 0.41
U^* = friction velocity ($m \, s^{-1}$)
ϕ_h = stability function for sensible heat
$\psi_m(\phi_m)$ = integrated momentum stability parameter as a function of ϕ_m
U_{CH} = wind velocity at the canopy height ($m \, s^{-1}$)

For agricultural applications, the canopy height is used as a reference height for calculating U*. The user is required to input the wind speed, at a height of 2 meters above the soil surface. The wind speed at the canopy height (U_{CH}) is computed based on the logarithm law:

$$\frac{U_{CH}}{U_{measured}} = \frac{\ln(\frac{Z_{CH} - \underline{D}}{Z_o})}{\ln(\frac{Z_{measured} - \underline{D}}{Z_o})} \tag{3-136}$$

The friction velocity U* can be visualized as a characteristic of the flow regime in the plant canopy compartment in which the logarithmic velocity distribution law holds. Rosenberg (1974) describes $Z_o+\underline{D}$ as the total height at which the velocity profile above the canopy extrapolates to zero wind velocity. The values for both Z_o and $\underline{D}$ can be estimated with the following procedures and equations presented by Thibodeaux (1979). For very short crops (lawns, for example), Z_o adequately describes the total roughness length, and little adjustment of the zero plane is necessary (i.e., D = 0). D is assumed to be zero in the current code when Z_{CH} is less than 5 cm. For tall crops, Z_o is related to canopy height (Z_{CH}) by

$$\log Z_o = 0.997 \log Z_{CH} - 0.883 \tag{3-137}$$

In tall crops Z_o is no longer adequate to describe the total roughness length, and a value of D, the zero plane displacement, is needed. For a wide range of crops and heights, $0.02 \text{ m} < Z_{CH} < 25 \text{ m}$, the following equation for D has been presented by Stanhill (1969):

$$\log \underline{D} = 0.9793 \log Z_{CH} - 0.1536 \tag{3-138}$$

This equation results from a linear regression analysis based on the published data for nineteen different crops with limited data measured for the same crop at different growth stages.

With estimates of Z_o and D, U* (friction velocity) can be estimated if the values of the stability parameters (ψ_m and ϕ_h) are known. These two variables are closely related to Ri, the Richardson number, which is the measure of the rate of conversion of convective turbulence to mechanical turbulence. It is defined as follows (Wark and Warner 1976):

$$Ri = \frac{(g/T)\ (\partial T/\partial Z)}{(\partial U\ /\ \partial Z)^2} \tag{3-139}$$

where

g = acceleration of gravity (m sec^{-2})
T = potential temperature (^{o}K)
Z = elevation (m)
U = wind velocity (m s^{-1})

Potential temperature is defined as the temperature which a parcel of dry air would acquire if brought adiabatically from its initial pressure to a saturated pressure of 1000 millibars (Perkins 1974). In application of the model, the measured temperature is used in the Richardson number estimation as suggested by Rosenberg (1974).

The sign of Ri indicates the atmospheric condition, and its magnitude reflects the degree of the influence. There are several different formulae for relating Ri to the atmospheric stability parameters; for these purposes, the sign of Ri is of greater concern than its magnitude. When Ri is larger than 0.003, the atmosphere exhibits little vertical mixing, reflecting stable conditions; when the absolute value of Ri is less than 0.003, neutral stability conditions exist (Oliver 1971); and when Ri is less than -0.003, convective mixing becomes dominant and atmospheric conditions are unstable.

To relate the atmospheric stability parameters to the Richardson number, Thom et al. (1975) proposed the following formulas based on the work by Dyer (1974) and Dyer and Hicks (1970):

For stable conditions

$$\phi_h = \phi_m = 1 + 5.2\ Ri \qquad (3\text{-}140)$$

For unstable conditions

$$\phi_h = \phi_m^2 = (1 - 16\ Ri\ )^{-1/2} \qquad (3\text{-}141)$$

For neutral conditions

$$\phi_h = \phi_m = 1 \qquad (3\text{-}142)$$

The integrated momentum stability parameter, ψ_m can be evaluated based on the following equation as derived by Lo (1977):

$$\psi_m = \frac{\pi}{2} - 1 + \ln 8 + \phi_m + 3 \ln \phi_m - 2 \ln(\phi_m + 1) - \ln(1 + \phi_m^2) - 2 \tan^{-1} \phi_m \qquad (3\text{-}143)$$

Under neutral conditions, $\psi_m = 0$ and the equation is not used.

In the application of these procedures, the calculations are performed as follows:

1) Evaluate Richardson number from temperature and wind velocity gradients.

2) Determine stability condition based on calculated Ri.

3) Calculate ϕ_h and ϕ_m, based on the stability condition and associated equations (3-130), (3-131) or (3-132).

4) Calculate ψ_m, from equation (3-133).

5) Calculate Z_o and $\underline{D}$ from canopy height using equations (3-127) and (3-128).

6) Estimate $K_z(Z)$, by applying equations (3-125), (3-124), and (3-123).

The resistance approach for the estimation of volatilization flux from the plant canopy--The calculation of the volatilization flux from the plant canopy is based on a resistance-type approach using the values of K_z

discussed above. For pre-plant pesticides, and time periods just after emergence and post-harvest, transport by volatilization from plant surfaces is much less than vapor phase transport by other mechanisms. For those conditions in which the plant leaves do not act as significant sources or sinks for pesticide vapor, the resistances of the air for the whole plant compartment can be estimated as follows (Mehlenbacher and Whitfield 1977):

$$\Sigma R = R_{bd} + R_{pc} \qquad (3\text{-}144)$$

$$R_{bd} = \frac{d}{D_a} \qquad (3\text{-}145)$$

$$R_{pc} = \int_{\underline{d}}^{Z_{CH}} \frac{dz}{K_z(Z)} \qquad (3\text{-}146)$$

where

ΣR = total vertical transfer resistance (day cm^{-1})
R_{bd} = boundary layer resistance (day cm^{-1})
$\underline{d}$ = thickness of the stagnant boundary layer (cm)
D_a = diffusion coefficient in air (cm^2 day^{-1})
R_{pc} = plant canopy resistance (day cm^{-1})

The flux is calculated as follows:

$$J_{pc} = AC_{gs}/\sum R \qquad (3\text{-}147)$$

where

J_{pc} = volatilization flux from plant canopy (g day^{-1})

C_{gs} = pesticide vapor concentration at the soil-atmosphere interface

The average concentration of pesticide vapor within the plant canopy is then given by summing the vapor fluxes into (due to soil, pond volatilization) and out of the plant canopy:

$$C_{CAN}^{t+1} = C_{CAN}^{t} + (J_{GD} + J_{pv} - J_{pc})/(Z_{CH}) \qquad (3\text{-}148)$$

where C_{CAN}^{t} is the concentration of vapor in the plant canopy at the start of the daily TFAT time step (g cm^{-3}) and C_{CAN}^{t+1} is the concentration at the end of the daily step (g cm^{-3}).

Soil Temperature Simulation--

Soil temperature is modeled in order to allow the program to calculate a temperature gradient for the Richardson number. The Richardson number is required so that atmospheric stability information can be passed to the FSCBG model.

Although a number of good models are available to calculate an energy balance at the soil surface to obtain the soil surface temperature and subsequently calculate soil profile temperatures, it was thought to be premature to go to this level of detail in TEEAM. Therefore, a regression type model is used to calculate the soil surface temperature of the form

$$T_b = A + BT_a \qquad (3\text{-}149)$$

in which

T_b is the soil surface temperature (°C)
T_a is the ambient air temperature (°C) and
A and B are regression coefficients.

Regressions on actual air and soil surface temperature data indicate that the linear relationship is quite adequate to provide this prediction on a monthly basis. Over the course of a day, it is suspected that the relationship would also hold.

Pesticide Granules--

In addition to soil and aerial applications, pesticide may also be applied to the soil surface in the form of pesticide granules. Granules are often applied as a means of controlling or slowing the release of pesticide into the environment, and may consist of kaolin, biodegradable polymers, or numerous other substances. Pesticides are incorporated into the granules by impregnation of preformed granules, coating of nonadsorbent granules, or extrusion of a mixture of granule medium and pesticide. The release of pesticide from granules may occur by one or more of the following mechanisms:

- Dissolution of the granule by rain or ponded water
- Diffusion and leaching of pesticide through the granule pore structure
- Leaching of pesticide from coated granule surfaces
- Volatilization of pesticide (i.e., vapor movement)

The relative importances of these release mechanisms will depend upon properties of the pesticide (vapor pressure, solubility, erodibility), properties of the granule medium (pore structure, erodibility), the method by which pesticide is incorporated into the granule, and environmental conditions (rainfall, temperature). Animals are exposed to granule-applied pesticide by either direct ingestion of granules or through the release of granule pesticide into soil and ponds.

Because the release of pesticide from granules varies greatly depending upon the granule formulation, there is as yet no general physically-based model of the fate of granules in agricultural fields. The release of pesticide from granules in TFAT is therefore modeled using a first order rate equation. The change in granule pesticide concentration over time is then given by:

$$\frac{dC_{GR}}{dt} = -K_{GR}\, C_{GR} \qquad (3\text{-}150)$$

where

C_{GR} = the concentration of pesticide in granules (g g^{-1})

K_{GR} = a granule rate constant ($days^{-1}$)

Integrating the above equation with respect to time yields the form used by TFAT to calculate granule concentrations and release rates:

$$C_{GR}^{t+1} = C_{GR}^{t}\, \exp(-k_{GR}\Delta T) \qquad (3\text{-}151)$$

where

C_{GR}^{t} = the concentration of pesticide in granules at the start of the day (g g^{-1})

C_{GR}^{t+1} = the granule pesticide concentration of the end of the day (g g^{-1})

ΔT = the daily TFAT time step, equal to one day

The mass of pesticide released to the soil surface during the TFAT time step is calculated as:

$$L_{GR} = C_{GR}^{t} M_{GR}\, (1-\exp(-K_{GR}\Delta T)) \qquad (3\text{-}152)$$

where

L_{GR} = the mass of pesticide released from granules (g)
M_{GR} = the total mass of applied granules (g)

The rate constant K_{GR} will obviously depend upon both the granule formulation and environmental conditions. To reflect the dependence of release rates on moisture conditions, K_{GR} is estimated as a weighted average of a fully saturated rate constant and a dry rate constant:

$$K_{GR} = \left(\frac{\theta}{\theta_s}\right)K_{wet} + \left(1-\frac{\theta}{\theta_s}\right)K_{dry} \qquad (3\text{-}153)$$

where

θ = the water content in the top soil (cm^3 cm^{-3})
θ_s = the saturated water content in the top soil layer (cm^3 cm^{-3})

K_{wet} = the release rate constant for granules immersed in water ($days^{-1}$)
K_{dry} = the release rate constant for dry granules ($days^{-1}$)

Thus, the granule release rate constant K_{GR} is recalculated at the start of each TFAT daily time step to reflect current moisture conditions. The rate of release will range from a rapid "wet" rate when moisture levels are high to a slower dry rate (i.e., due to volatilization) during dry periods. Note that it is assumed that moisture conditions for the granule can be represented by the degree of saturation in the surface soil layer.

3.3 PLANT GROWTH MODULE (PLTGRN)

3.3.1 Introduction

Plant growth can be viewed as an ancillary ecosystem process which must be simulated in order to predict the uptake and translocation of pesticides or other xenobiotics from the soil, either to estimate exposure to herbivores or to predict direct effects on plants themselves.

Plant growth is difficult to describe mathematically, as it is a complex function of the interaction between many chemical, physical, and climatic factors, including moisture availability, nutrient availability, temperature, radiation, soil texture, and plant physiological features. The change in plant biomass with these factors is necessary information for the toxicant application module (for simulating the effect of plant canopy on deposition), the soil fate and transport module (for simulating the effect of roots on water movement), the plant contaminant translocation module (for estimating the toxicant burden in plant biomass), and the terrestrial areal exposure module (for estimating the available plant biomass, both contaminated and uncontaminated, for ingestion).

In PRZM Release 1 there was a simple model which simulates plant growth as a linear function of time. Plant parameters, including canopy areal development, plant biomass, and root depth, are assigned initial values, usually zero, at emergence and take on maximum values at maturity. At all intervening times, plant parameter values are weighted by the fraction of the growing period that has elapsed.

This plant growth model has been replaced in TEEAM. The motivation is that, at a later date, environmental conditions and the presence of toxicants which may affect plant growth can be accounted for. This cannot be done with the current model. The plant growth module used is a relatively simple model which is applicable to a variety of plants, both annuals and perennials. The model is based on the crop growth formulation developed for the USDA's Erosion-Productivity Impact Calculator (EPIC). The documentation for EPIC is in draft form and the actual FORTRAN code is unclear, with few comments describing its operation; as a result, the code used in TEEAM was rewritten from previous articles describing EPIC (Williams et al. 1983; Williams et al. 1987).

3.3.2 Development of TEEAM Plant Growth Module as Adapted from EPIC

The EPIC plant growth model predicts potential biomass increase as a function of solar radiation, leaf area index (LAI), and hours of available sunlight. Actual biomass increase is the potential biomass increase reduced by growth regulating factors: temperature stress, water stress, and nitrogen or phosphorus limitation. The TEEAM version of this model currently considers only temperature stress.

The potential growth rate is defined by the equation:

$$\frac{d(B_p)}{dt} = (BE)\ (PAR) \qquad (3\text{-}154)$$

where

B_p = potential biomass (kg ha^{-1})

BE = crop-specific parameter for converting energy to biomass (kg m^2 MJ^{-1} ha^{-1} day^{-1})

PAR = photosynthetic active radiation (MJ m^{-2})

The photosynthetic active radiation is computed once each day utilizing the formula:

$$PAR = 0.02092\ (RA)\ \{1 - \exp[-0.65\ (LAI + 0.05)]\} \qquad (3\text{-}155)$$

where

RA = solar radiation (ly)

LAI = field level leaf area index (decimal)

The leaf area index is also computed at the start of each day. It is a function of the computed biomass and asymptotically approaches a maximum value in the growing season after which it starts to decline. This is expressed by the following relation:

$$LAI = \begin{cases} \dfrac{(LAI_{mx})\ (WLV)}{WLV + 5512 \exp\ [-0.000608\ (WLV)]}, & B_1 \leq DLAI \\[2ex] LAI_o \left(\dfrac{1 - B_1}{1 - DLAI}\right)^2, & B_1 > DLAI \end{cases} \qquad (3\text{-}156)$$

where

LAI_{mx} = maximum potential leaf area index (dimensionless)
WLV = aboveground biomass minus yield (kg ha^{-1})
LAI_o = leaf area index when B_1 equals DLAI (decimal)
B_1 = dimensionless expression of accumulated biomass (fraction)
DLAI = fraction of growing season after which LAI begins to decline (fraction)

This relationship is plotted for the case of $B_1 <$ DLAI in Figure 3.7. As the plot demonstrates, LAI reaches 90% of LAI_{mx} when WLV is approximately 4100 kg/ha. This relationship is utilized for all crops; the only crop-specific parameters in this relationship are LAI_{mx}, the maximum leaf area index, and DLAI, the fraction of the growing season when LAI begins to decline.

The variable B_1 is calculated as a function of accumulated degree days:

$$B_1 = \sum_{i=1}^{n} \frac{HU}{PHU} \tag{3-157}$$

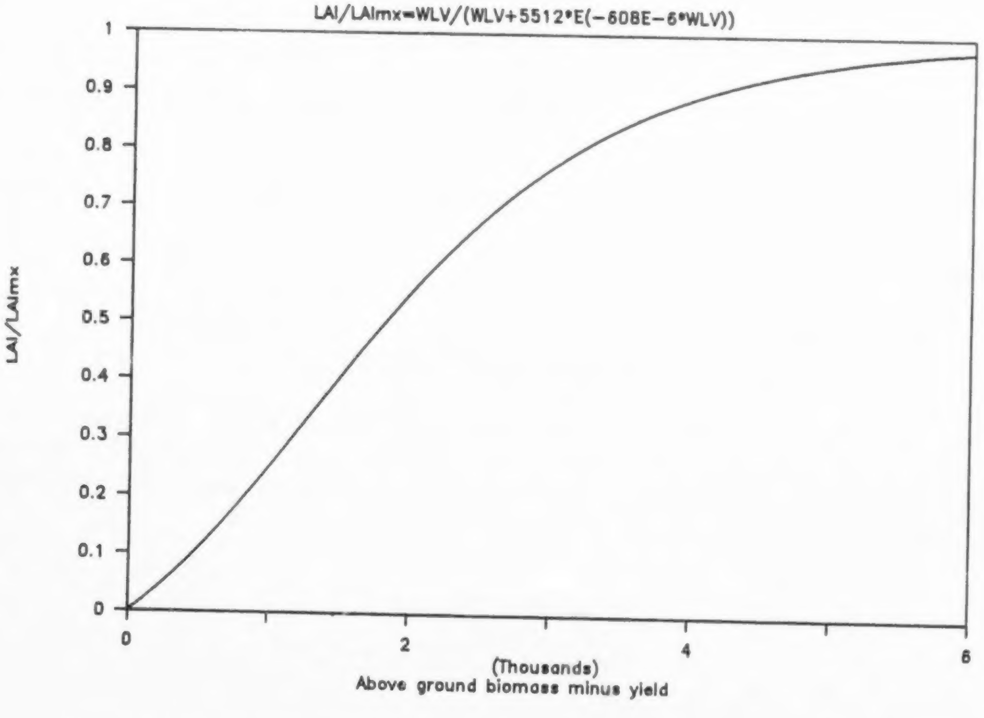


Figure 3.7 Leaf area index as a function of above-ground biomass minus yield.

where

HU = heat unit (°C day)
= $(T-T_b)$ (1 day) if T (the average air temperature, °C, for the day) is greater than T_b (a user specified base temperature, °C)
PHU = parameter for crop specifying the (potential) heat units necessary for maturation (°C day)
n = number of days

The value of WLV is computed daily using the relation:

$$WLV = B_p - RWT - YLD \tag{3-158}$$

where

RWT = root biomass (kg ha^{-1})

YLD = crop yield (kg ha^{-1})

Change in yield is computed with the relation:

$$\frac{d(YLD)}{dt} = \frac{d(B_p)}{dt} \frac{B_1}{(GK)} \tag{3-159}$$

where

GK = ratio of total biomass to crop yield under favorable growing conditions (decimal)

Root growth is computed with:

$$\frac{d(RWT)}{dt} = \frac{d(B_p)}{dt} \left(0.4 - 0.2\ B_1\right) \tag{3-160}$$

Root depth is another variable necessary for the TFAT module. It is computed with the relationship:

$$\frac{d(DPTH)}{dt} = 2.0\ (RZ)\ (HU)/(PHU),\quad DPTH < RZ \tag{3-161}$$

where

DPTH = root depth (cm)
RZ = crop-specific maximum root depth (cm)

Finally, the actual plant growth is the potential biomass increase reduced by the growth regulating factor:

$$\frac{d(B)}{dt} = \frac{d(Bp)}{dt} REG \qquad (3\text{-}162)$$

where

B = actual biomass (kg ha^{-1})
REG = growth regulation factor (fraction)

REG is also used to reduce the rates of YLD, RWT, and DPTH increase.

In the TEEAM version, REG is only a function of temperature stress:

$$REG = \exp\left\{\Omega\left[\frac{T_o - T}{T}\right]^2\right\} \qquad (3\text{-}163)$$

where

Ω = temperature stress parameter for the crop (decimal)
T_o = optimal air temperature for the crop (°C)
T = daily average air temperature (°C)

The temperature stress parameter is computed from user-supplied temperatures representing the optimal growing temperature (T_o) and a minimum (base) temperature at which the plant can grow:

$$\Omega = \frac{\ln(0.9)}{\left[\frac{T_o - \bar{T}}{\bar{T}}\right]^2} \qquad (3\text{-}164)$$

where

$\bar{T}$ = the mean of the optimal temperature (T_o) and base temperature (T_b) (°C)

$$= \frac{T_o + T_b}{2}$$

The EPIC plant growth model also includes the simulation of the weight distribution of roots with depth. This additional variable is not currently simulated in TEEAM, but may be added easily if water stress is considered in future versions.

3.3.3 EPIC Modifications for Inclusion in TEEAM

The model described above is, in modified form, included as the TEEAM subroutine PLTGRN. PLTGRN returns the following variables to TEEAM for subsequent calculations: plant above ground biomass (kg m^{-2}), root biomass (kg m^{-2}), root depth (cm), canopy cover (fraction), and canopy height (m). Plant above ground biomass is computed as a straightforward transformation of the computed total plant biomass minus the root weight:

$$WEIGHT = (B - RWT)/10{,}000 \qquad (3\text{-}165)$$

The root biomass used in subsequent TEEAM calculations is the live root biomass calculated within PLTGRN converted from kg ha^{-1} to kg m^{-3}:

$$ROOTWT = RWT/10{,}000 \qquad (3\text{-}166)$$

The root depth is passed directly to TEEAM from PLTGRN since the units are the same in both code sections (m).

Canopy cover is computed from the following function (a logistic function) of leaf area index (LAI):

$$COVER = COVMAX/[1.0 + \exp(4.61 - 3.07\ LAI)] \qquad (3\text{-}167)$$

where:

COVER = fraction of ground covered by the plant
COVMAX = crop specific maximum cover

This function was selected since it approximated (Figure 3.8) the relationship described in the PRZM documentation (Carsel et al. 1984)

$$COVER = [2.0 - Erfc\ (1.33\ LAI - 2.0)]/2.1 \qquad (3\text{-}168)$$

where:

Erfc = complementary error function

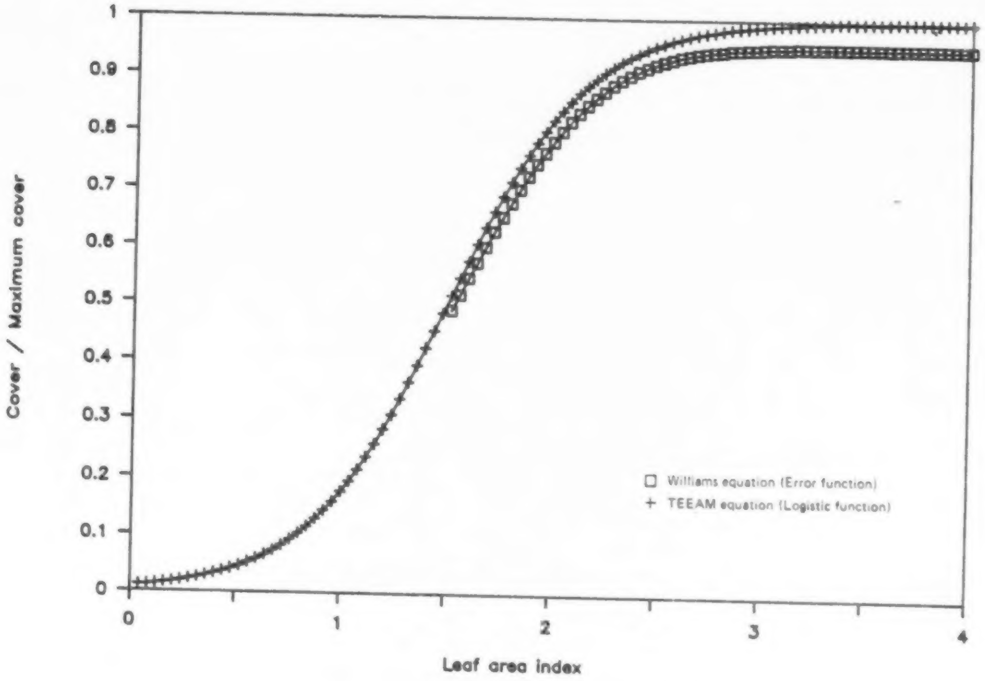
Equation 3-167 is used rather than 3-168 since values for COVER are required for values of LAI less than 1.0 (Equation 3-168 is not defined for values of LAI less than 1.5). LAI as computed within PLTGRN is a field level value, e.g., the amount of leaf area in a field per area of the field, and can have values less than 1.0.

Canopy height is not computed as part of EPIC. For the TEEAM plant growth model, the EPIC rooting depth equation was adapted to simulate canopy height over time:

$$\frac{d(HEIGHT)}{dt} = (KHGT)\ (REG)\ (HU)/(PHU), \quad HGT < HGT_{mx} \qquad (3\text{-}169)$$

where

HGT = canopy height (m)
KHGT = crop-specific maximum rate of height increase (day^{-1})
HGT_{mx} = crop-specific maximum potential height (m)



Figue 3.8 Cover as a function of leaf area index.

3.4 PLANT CONTAMINANT TRANSPORT MODULE (PLTRNS)

3.4.1 Introduction

This submodel simulates contaminant transport within plants of the simulated ecosystem. It is necessary to simulate this process to determine the quantity of contaminant which enters the plant biomass and to determine the concentrations of contaminant within various types of plant tissue. These concentrations can then be used in determining detrimental effects to the plants and to determine the concentrations in plant tissues which may form part of the diet of the herbivores and omnivores of the simulated ecosystem. To simulate the total concentration of contaminant within and on plants, it is necessary to determine the rate of uptake of the contaminant through the root system and to determine both the amount of contaminant which is deposited on and remains on the aboveground plant matter after toxicant application to the ecosystem.

Ultimately, it would be preferable to simulate the plant tissues which might be preferentially eaten by the animals in the simulated ecosystem (e.g., leaves, fruit, seeds, stems, and roots). At the current time, however, the plant contaminant transport model only simulates aboveground and root biomass concentrations. There is the inherent assumption that all plant material which is aboveground has the same contaminant concentration regardless of the plant tissue types which might be involved. (Similarly, all root tissues would have an associated "root concentration" which would be the same for all roots.)

3.4.2 Background

A plant contaminant transport model (UTAB) being developed at Oregon State University (Boersma et al., in press) was evaluated for its potential use as a module within TEEAM. In this evaluation it was determined that, in its current state, UTAB would be overly complex (requiring too many input parameters and not commensurate with the level of detail of the plant growth model) to be used in the TEEAM structure. However, at a later date, it may be appropriate to link this model into the TEEAM framework.

Instead, a relatively simple model which has readily available parameters which determine the amount of contaminant being transported into the roots and the amount passing from the roots to the aboveground structure has been implemented. This model is based upon the experimental work of Briggs et al. (1982) relating the rates of root uptake and translocation to the lipophilicity of the applied contaminant.

3.4.3 Development of Module

The model has two-compartments; the contaminant flows into the roots from the soil solution and flows into the aboveground biomass from the roots (Figure 3.9). The root compartment is simulated as a completely mixed reactor. The input to the roots is the soil solution concentration times the flow rate reduced by a reflection coefficient (R_w) representing the resistance of the root surface to the chemical. Within the roots, the contaminant can degrade at a user-specified first order rate (λ). The contaminant leaves the root through the transpiration stream leading to the aboveground biomass. This rate of transfer is governed by a root/aboveground biomass reflection coefficient (R_r).

The aboveground biomass compartment is simulated as having two phases, an aqueous and a nonaqueous phase. The transfer between these phases is governed by a partition coefficient (K_p). The contaminant can decay within this compartment at the same rate as specified for the roots. The contaminant can leave the aboveground biomass to the atmosphere governed by an aboveground biomass/atmospheric reflection coefficient (R_e).

The mass balance equation for plant roots is written as:

$$M_r \frac{dC_r}{dt} = R_w C_w Q_r - R_r C_r Q_t - \lambda C_r M_r \qquad (3\text{-}170)$$

in which

M_r = the total weight of plant roots (wet basis) (g)

C_r = the concentration of contaminant in the roots (g g^{-1})

R_w = a reflection coefficient for contaminant transfer from the soil solution to the root (decimal)

C_w = the concentration of contaminant dissolved in the soil solution (g cm^{-3})

Q_r = the flow into the root biomass (cm^3 day^{-1})

R_r = a reflection coefficient for contaminant transfer from the root to the aboveground transpiration stream (g cm^{-3})

Q_t = the flow rate into the stem xylem (cm^3 day^{-1})

λ = the first order degradation rate of the chemical in the plant tissue (day^{-1})

The first term on the right-hand side represents the gain to the roots from the soil solution; the second, the loss to the aboveground biomass; and the third, internal degradation.

For the purpose at hand, the flow rate Q_r and Q_t are assumed to be equal, indicating no change in water storage within the plant. These flow rates are the product of a velocity and a cross-sectional area within various portions of the plant. The velocity is defined throughout the plant to be uniform and equal to TDET, the evapotranspiration rate given by TFAT

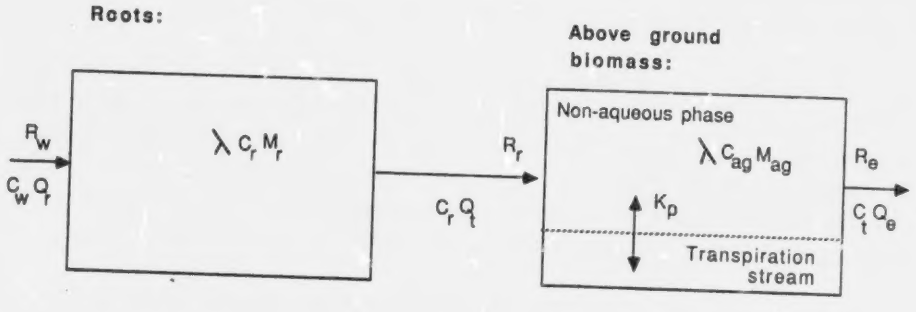


Figure 3.9 Schematic of plant contaminant transport module (PLTRNS).

(cm day^{-1}). Therefore, to maintain continuity of flow, A_r and A_t, the respective cross-sectional areas of flow in the roots and plant tops, must be equal. Since TFAT simulates vertical transfers of water and contaminant for a unit area (cm^2) these areas must also take on that dimension.

In reality, the velocity of water movement changes greatly in the plant due to variation in cross-sectional flow area and losses/changes in storage which actually occur. In order to maintain simplicity, constant velocity and flow areas have been utilized.

At steady-state conditions and with the assumption of no internal decay, Equation (3-167) reduces to:

$$\frac{C_r}{C_w} = \frac{R_w}{R_r} \tag{3-171}$$

This ratio is equal to the root concentration factor (RCF, with units of ml (or cm^3) of external solution divided by the mass of roots in grams) as defined by Briggs et al. (1982). Thus, the root/aboveground transpiration stream reflection coefficient can be expressed in terms of RCF and the root uptake reflection coefficient:

$$R_r = \frac{R_w}{RCF} \tag{3-172}$$

The assumption of no internal decay is valid for the above analysis since, in the experimental determination of RCF, degradation had been accounted for.

Using the above relationship; the fact that $Q_r = Q_t = (TDET)\ A$, where A is the total area of the simulated ecosystem; and dividing both sides of Equation (3-170) by M_r, the following relationship is obtained:

$$\frac{dC_r}{dt} = \frac{R_w\ C_w\ TDET\ A}{M_r} - \frac{R_w\ C_r\ TDET\ A}{RCF\ M_r} - \lambda C_r \tag{3-173}$$

The ratio of M_r to A is the root biomass density simulated by the PLTGRN module. C_w and TDET are simulated by the TFAT module. Given values of R_w, RCF, and λ , Equation (3-173) can be solved numerically.

The mass balance for the contaminant in the aboveground biomass can be written as:

$$M_{ag}\frac{dC_{ag}}{dt} = R_r C_r Q_t - R_e C_t Q_e - \lambda C_{ag} M_{ag} \tag{3-174}$$

where

M_{ag} = the total weight (wet basis) of the aboveground biomass (g)

C_{ag} = the concentration of contaminant in the aboveground biomass ($g\ g^{-1}$)

R_e = the reflection coefficient for transfer to the atmosphere (decimal)

C_t = the concentration of contaminant in the transpiration stream ($g\ cm^{-3}$)

Q_e = the flow of water into the atmosphere ($cm^3\ day^{-1}$)

As with the root compartment, no change in water storage is simulated so that $Q_t = Q_e =$ (TDET) A.

Solving Equation (3-174) for steady state and with similar reasoning as previously described, assuming no internal decay, produces:

$$\frac{C_t}{C_r} = \frac{R_r}{R_e} \tag{3-175}$$

The ratio of C_t to C_w is defined by Briggs et al. (1982) as the transpiration stream concentration factor (TSCF, with units of ml of external solution divided by mass of water in the transpiration stream in grams).

Using this definition of TSCF and the previous definition of RCF, Equation (3-173) can be rewritten:

$$\frac{R_r}{R_e} = \frac{TSCF}{RCF} \tag{3-176}$$

Given this and the relation obtained in Equation (3-171), R_e can be written as a function of R_w:

$$R_e = \frac{R_w}{TSCF} \tag{3-177}$$

Using this relationship, the assumption of no change in internal water storage, and dividing Equation (3-173) by M_{ag} produces:

$$\frac{dC_{ag}}{dt} = \frac{R_w\ C_r\ TDET\ A}{RCF\ M_{ag}} - \frac{R_w\ C_t\ TDET\ A}{TSCF\ M_{ag}} - \lambda C_{ag} \tag{3-178}$$

The only undefined component in the above equation is C_t, the concentration of contaminant in the aqueous phase (transpiration stream). A mass balance of the two phases within the aboveground biomass compartment can be written as:

$$M_{ag}C_{ag} = V_tC_t + m_{na}C_{na} \qquad (3\text{-}179)$$

where

V_t = volume of the aqueous phase (cm^3)
m_{na} = mass of the nonaqueous phase (g)
C_{na} = the concentration of contaminant in the nonaqueous phase ($g\ g^{-1}$)

By defining the following parameters, assumed to be constant for a plant/contaminant combination:

ϕ_a = aboveground biomass water content ($cm^3\ g^{-1}$) [or equivalently, for water ($g\ g^{-1}$)]
K_p = partition coefficient for plant, the ratio of the concentration in the nonaqueous phase to the concentration in the aqueous phase ($cm^3\ g^{-1}$)
ρ_{na} = ratio of the mass of the nonaqueous aboveground biomass (dry weight) to the total aboveground biomass (wet weight) ($g\ g^{-1}$) (essentially, the percent dry matter)

C_t can be written in terms of C_{ag} using Equation (3-177):

$$C_t = C_{ag}/(\phi_a + K_p\rho_{na}) \qquad (3\text{-}180)$$

Given this relationship, Equation (3-172) can be solved numerically for C_{ag}.

In the plant translocation module the root and aboveground concentrations C_r and C_{ag} are computed by a finite difference solution of Equations (3-175) and (3-180). A backwards difference scheme is used to approximate the time derivatives:

$$\frac{dC_r}{dt} \approx \frac{C_r^{t+1} - C_r^t}{\Delta T} \qquad (3\text{-}181)$$

$$\frac{dC_{ag}}{dt} \approx \frac{C_{ag}^{t+1} - C_{ag}^t}{\Delta T} \qquad (3\text{-}182)$$

where the superscript t refers to values at the start of the daily time step ΔT, and t+1 refers to end of time step values. Equations (3-173) and (3-178) are then written in finite difference forms:

$$\frac{C_r^{t+1} - C_r^{t}}{\Delta T} = \frac{R_wC_w^{t+1}\text{TDET } A}{M_r^{t+1}} - \frac{R_wC_r^{t+1}\text{TDET } A}{\text{RCF } M_r^{t+1}} - \lambda C_r^{t+1} \qquad (3\text{-}183)$$

$$\frac{C_{ag}^{t+1} - C_{ag}^{t}}{\Delta T} = \frac{R_w C_r^{t+1} \text{TDET A}}{\text{RCF } M_{ag}^{t+1}} - \frac{R_w C_t \text{ TDET A}}{\text{TSCF } M_{ag}} - \lambda C_{ag}^{t+1} \qquad (3\text{-}184)$$

All of the terms in the above equations are known at the end of the time step except for C_r^{t+1} and C_{ag}^{t+1}. Because Equation (3-182) contains the root zone concentration, Equation (3-183) is solved first for the new value of C_r^{t+1}. C_{ag}^{t+1} can then be determined explicitly from Equation (3-184).

The parameters TSCF (transpiration stream concentration factor) and RCF (root concentration factor) are expressed as functions of K_{ow} by Briggs et al. (1982):

$$\log (\text{RCF} - 0.82) = 0.77 \log K_{ow} - 1.52 \qquad (3\text{-}185)$$

$$\text{TSCF} = 0.784 \exp - \left[(\log K_{ow} - 1.78)^2/2.44\right] \qquad (3\text{-}186)$$

in which K_{ow} is the octanal/water partition coefficient.

Obviously, major biochemical processes are ignored in this model. Descriptions of these processes are lumped into the empirical coefficients such as TSCF and RCF.

3.5 TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM)

3.5.1 Introduction

In preceding sections, we have described the simulation of toxicant movement within the soil/plant/atmosphere systems. These systems provide the vectors for toxicant uptake by ecosystem fauna. This section describes the processes through which animals are exposed to and accumulate the toxicants.

Once the toxicant concentrations in the environment are known, two factors control accumulation: (1) the presence of the animal in areas where the toxicant is present and (2) the uptake of the toxicant into the body of the animal. Unlike plants, animals enjoy varying degrees of freedom in their movement. Therefore, if they are capable of detecting the toxicant they may avoid or be attracted to contaminated areas. Even in the absence of a toxicant, animals may move preferentially to various portions of their habitat. Factors which affect their movement include loss of habitat, predator avoidance, seasonality, and food search. Even though their movements are certainly determined by environmental and species-specific behavioral factors, there is also an inherent degree of randomness in their movements within their home range.

The second factor in evaluating accumulation is the uptake of the toxicant into the animal's body tissues. Figure 3.9 demonstrates potential routes of exposure. The animal may ingest a number of contaminated vectors: water (i.e., ponded water at the soil surface), soil, living or dead plant material, pesticide granules, or living prey. In certain species, vapor-phase toxicants or chemicals adsorbed to particulates may be inhaled. Other species may absorb chemicals through dermal contact with contaminated soil or water. The magnitude of uptake via these routes will obviously be species- and chemical-dependent.

Once the chemical is taken into the animal's body, it may accumulate in various organs, metabolize, filter through the endocrine system (in higher animals) or leave the body through elimination. Depending upon the species, elimination may occur through the skin or in excreted wastes. Death of the organism and subsequent decay of the body materials will ultimately return the chemical to the soil. Organ-specific accumulation and return to the soil, via mortality and decay, are not considered in this model.

3.5.2 Module Development

The terrestrial food chain model consists of three principal components: (1) animal movement, (2) animal feeding, and (3) toxicant assimilation. The animal movement component determines how often animals come into contact with soil, prey, and other sources of toxicant contamination. The animal feeding component calculates the mass of food ingested by animals, and the toxicant assimilation component determines how much toxicant is assimilated into body tissues from ingested food and other sources. The model currently assumes that population levels are at steady-state; an additional component can be added at some future time to simulate birth and death rates.

3.5.2.1 Animal Movement--

The location and movement of animals are major factors in determining exposure. Unfortunately, there appear to be few simulation models which describe animal movements. In the absence of more species-specific or detailed models, a simple Markov model is used to move animals among environmental compartments. This type of model allows for a degree of randomness in the movement of the animals with respect to the toxicant. Realistically, animals are not uniformly or continuously exposed and such a model will account for this fact.

The Markov model moves animals among habitats, or within a habitat among soil horizons, based on the animal's current location and a transition probability matrix. Soil animals move among soil horizons, while higher order predators move between habitats. The transition probability is simply the probability that the animal will emigrate to location "b" given that it is currently in location "a". Several such matrices could be input and used to vary the movement of animals on a seasonal or life-stage basis or in consideration of modification of behavior triggered by various environmental conditions.

Mathematically, the state of such a system at time 't' is given by

$$p^{(t)} = p^{(t-1)}\underline{P} \qquad (3\text{-}187)$$

where p is a vector describing the location or distribution of the animal population, the superscript 't' denotes time, and the matrix $\underline{P}$ is a transition probability matrix.

The transition matrix, $\underline{P}$, contains elements f_{ab} defined by

$$f_{ab} = \text{Prob}\ (X_t = b|X_{t-1}=a) \qquad (3\text{-}188)$$

In other words, the probability that the organism is in a given location (b) depends upon its location (a) during the previous time step. $\underline{P}$ is an m x m matrix of the following form, where m is the number of possible locations:

$$\underline{P} = \begin{array}{lll} f_{11} & f_{12}\cdots\cdots & f_{1m} \\ f_{21} & & \\ \vdots & & \\ f_{m1} & & f_{mm} \end{array} \qquad (3\text{-}189)$$

and has the following property

$$\sum_b f_{ab} = 1 \qquad (3\text{-}190)$$

(Haan 1977).

The output of the model is a vector of probabilities $p_h^{(t)}$ or $p_c^{(t)}$. The p_h represent the probability that an animal is in a particular habitat (h) and the p_c refer to the probability that the animal will be in a given soil horizon (c) within a given habitat during a time 't'. Conservation of mass requires that

$$\sum_h p_h^{(t)} = 1 \qquad (3\text{-}191)$$

and

$$\sum_c p_c^{(t)} = 1 \qquad (3\text{-}192)$$

This model can be used in one of two ways; either to describe the random movement of a single individual or subpopulation moving en masse, or to describe the distribution of a population in time.

In the first mode of operation (en masse movement of animals) the probability that the animal moves to each possible new location is determined from the previous location of the animal and its Markov transition matrix. A uniform random number between 0 and 1 is generated to determine which habitat or soil horizon the animal (or animal subgroup) actually moves to. Although the location of the animal at any particular time is selected randomly, the transition matrix ensures that the animal will exhibit preferences for habitats and compartments with high transition probabilities.

The following example illustrates this first mode of operation. Suppose there are three distinct habitats of interest: a nesting area, a contaminated feeding area, and an uncontaminated feeding area. The transition matrix might look like the following:

$$P = a \begin{array}{c|ccc} & & b & \\ & 1 & 2 & 3 \\ \hline 1 & 0.50 & 0.25 & 0.25 \\ 2 & 0.70 & 0.25 & 0.05 \\ 3 & 0.25 & 0.25 & 0.50 \end{array} \qquad (3\text{-}193)$$

Reading the first row, the probability that the animal will be in habitat 1 given that it was in habitat 1 in the previous time step is 0.5. The probability that it will be in habitat 2 given that it previously was in habitat 1 is 0.25 and so forth.

Once the initial vector of the animal location ($p^{(t=0)}$) is given (habitat 1, 2, or 3) the matrix can be used to move the animal among habitats. Suppose the animal is initially located in habitat 1, so that

$$p^{(t=0)} = \begin{array}{c} 1 \\ 0 \\ 0 \end{array} \qquad (3\text{-}194)$$

A uniform random number between zero and one is then chosen. If the number chosen were 0.89, the animal would move to habitat 3 since 0.89 is >0.50 (f_{11}) and also >0.75 ($f_{12} + f_{11}$). At the next time step, another random number would be chosen and the animal would move based on the transition probabilities from habitat 3.

The elements of matrix $\underline{P}$ can be designed so that the animals may move in a completely random fashion (for instance all the f_{ab} very nearly equal) or completely deterministically (single non-diagonal f_{ab} on each row being unity).

The second mode of operation is to use the transition matrix to determine the distribution of a population among several habitats or soil horizons through time. Suppose the initial distribution among habitats is given by:

$$p^{(0)} = \begin{matrix} 0.67 \\ 0.20 \\ 0.13 \end{matrix} \qquad (3\text{-}195)$$

In this example, 67 percent of the population is in habitat 1, 20 percent is in habitat 2, and 13 percent is in habitat 3. The distribution of the population at the next time step is given by:

$$p^{(1)} = p^{(0)}\underline{P} \qquad (3\text{-}196)$$

In general, the distribution at time t is given by:

$$p^{(t)} = p^{(t-1)}\underline{P} \qquad (3\text{-}197)$$

As time becomes large ($t \rightarrow \infty$) the population distribution reaches a steady-state condition such that:

$$p^{(t)} = p^{(t-1)} \qquad (3\text{-}198)$$

Although it is felt that accounting for randomness in animal behavior is important in determining exposure, it seems equally important to be able to simulate more deterministic behavior patterns which may result in modification of exposure. Such behavior might include the following:

- Aggregation of animals at ephemeral ponds for drinking or bathing
- Saturated soil conditions which might cause earthworms to migrate to the soil surface
- Modification of feeding caused by extreme precipitation or temperature

An appropriate means of handling this within the framework of the proposed model would be to supply special transition matrices which would be used in conjunction with the occurrence of these environmental conditions. For instance, if the water content in a soil compartment goes to saturation, then the special transition matrix would reflect a high probability that earthworms would migrate to the surface of the soil. If the ambient air temperature is above a certain threshold, the transition matrix might reflect a high probability that a terrestrial mammal might not venture forth to feed. In the current version of the model, only one transition matrix can be input and behavioral responses to these special environmental conditions cannot be simulated.

3.5.2.2 Animal Feeding--

A wealth of information is available on food intake rates and food preferences for many of the species of interest on a seasonal or life-stage basis. Some examples of the literature can be found in Section 6.7.3. In lower trophic levels, animals may feed more or less continuously unless they are in their nesting habitat. Therefore, their total intake of food and the mixture of items may be fairly constant (given unlimited availability). In the upper trophic levels, animals (carnivores, raptors) may kill only intermittently. In this case the modeling is more involved. Factors may include location of predator relative to prey, time elapsed since the last kill and probability of prey capture. In addition, once a kill has been made the predator may devour only certain portions of the prey. In this case, modeling of the concentrations of toxicants in various organs of animals in intermediate trophic levels might be useful; however, this is not available in this version of TEEAM.

The feeding model assumes that an average daily food intake rate U^i_T can be established for each species. Here the superscript "i" denotes a given animal group or population. The total daily intake is broken down into the uptake of specific prey by means of preference factors. Thus the specific daily consumption of food item j by predator i under ideal predation conditions is

$$U^i_j = \beta^i_j \, U^i_T \tag{3-199}$$

β^i_j is a vector of food preference factors of species i for prey j, assuming that the availability of prey "j" is typical of that in an unstressed ecosystem. The β^i_j, must sum to unity. For instance, if the predator is a passerine bird and its ideal diet consists of 25% seeds (prey 1), 50% earthworms (prey 2), and 25% soil macroarthropods (prey 3), then the vector β^i would be

$$\beta^i = \begin{array}{cc} 1 & 0.25 \\ 2 & 0.50 \\ 3 & 0.25 \end{array} \tag{3-200}$$

Predator/prey relationships can be established in the model through the use of this vector. An entry of zero for any species "j" in the vector indicates that species "i" does not prey on species "j." Food items currently available in the model include other animals, plants, soil, ponded water, inhaled air, and pesticide granules.

Successful predation in higher-order animals depends upon two factors: that both predator and prey are brought into contact (i.e., are in the same habitat) and that the predator is successful at capturing the prey. The expression of this success in the model is accomplished by the use of probabilities. The daily consumption rate of food item j by predator i then becomes:

$$U_j^i = \beta_j^i \, U_T^i \sum_h p_{j/h}^i \, p_h^{ij} \tag{3-201}$$

where

U_j^i = feeding rate of predator i on prey j (mg/day)

$p_{j/h}^i$ = probability that predator i catches prey j given that both are in habitat h

p_h^{ij} = probability that predator i and prey j are both in habitat h

The probabilities that predator and prey are both in each habitat (p_h^{ij}) are determined from the Markov animal movement model. The capture probabilities $p_{j/h}^i$ are conditional probabilities which assume unlimited availability of prey.

Because it is unrealistic to allow animals to continue to feed after ingesting lethal dosages of toxicant, the feeding model decreases total uptake rates as a function of cumulative toxicant dosages:

$$U_T^i = K_f (U_T^i)^\circ \tag{3-202}$$

where

U_T^i = the current total uptake rate for animal group i (mg day^{-1})

$(U_T^i)^\circ$ = the initial uptake rate for animal group i when no toxicant has been ingested

K_f = uptake reduction factor computed as a function of cumulative dosage ($0 \leq K_f \leq 1.0$).

Dosage in this case is defined as the cumulative mass of toxicant ingested per unit biomass. In the current version of the model K_f is calculated as a linear function of dosage based on the 10 percent and 50 percent lethal dosages:

$$K_f = .9 - \frac{(.5 - .9)}{(\text{LD50} - \text{LD10})} \text{LD10} + \frac{(.5 - .9)}{(\text{LD50} - \text{LD10})} D^t \tag{3-203}$$

where

LD10 = the dosage of toxicant which is lethal to 10 percent of animals (g g^{-1})

LD50 = the dosage of toxicant which is lethal to 50 percent of animals (g g^{-1})

D^t = the cumulative toxicant dosage at time t (g g^{-1})

This assumes that at the LD10 , uptake is reduced by 10 percent (i.e., 10 percent of the animal group is dead) while at the LD50, uptake is reduced by 50 percent. At zero dosage the uptake factor K_f is set to 1.0 to indicate that uptake is unaffected by toxicant ingestion. In addition, if the calculated value of K_f is greater than unity or less than zero, the program defaults the value to the appropriate limit.

If a population model which accounts for mortality due to toxic effects is ultimately coupled with this model, the factors $p^i_{j|h}$ and β^i may be altered depending upon the abundance of prey and the use of the uptake reduction factor (K_f) could be eliminated. In order for the system to be stable the condition

$$M_o^j > U_j^i \, \Delta t \tag{3-204}$$

must be satisfied, where M_o^j is the total biomass of species j during the time step Δt. Simply stated, the intake rate by predator "i" of prey "j" cannot exceed the total biomass of prey "j."

3.5.2.3 Toxicant Assimilation--

Toxicant assimilation within the organism is a complex process affected by the following factors:

- The biochemistry and physiology of the specific species of interest
- The properties of the chemical (e.g., lipophilicity)

Because of the complexity of the processes involved, the modeling approach must at this time be empirical. Since Corvallis ERL personnel are ultimately to provide models for the fate of toxicants within the animal species of interest, the intent is to implement a set of very simple algorithms in the prototype model which would apply to idealized species. These simple models will ultimately have default parameter values which will provide the capability to simulate broad differences among species in toxicant assimilation and subsequent body burden.

The mass of toxicant present in the biomass of a group of animals will vary over time due to assimilation, metabolic degradation, and predation by other animals. The mass balance equation for toxicant in each individual animal, subgroup, or population is therefore written mathematically as:

$$\frac{d\,(M_o^i \; C_o^i)}{dt} = J_a^i - J_d^i - J_p^i \tag{3-205}$$

where

M_o^i = biomass of animal group i (mg)

C_o^i = concentration of toxicant in animal group i (mg mg^{-1})

J_a^i = toxicant assimilation rate (mg day^{-1})

J_d^i = toxicant degradation rate for animal group i (mg day^{-1})

J_p^i = toxicant predation loss rate (mg day^{-1})

Toxicant assimilation will depend upon the rate at which toxicant is ingested and the rate at which ingested toxicant is absorbed into the tissues of the animal. The rate at which toxicant is ingested by animal group i when it preys on food item j is given by the product of the feeding rate U_j^i (Equation 3-197) and the toxicant concentration in food items:

$$F_{ij} = C_o^j \beta_j^i U_T^i \sum_h p^i_{j|h} p_h^{ij} \qquad (3\text{-}206)$$

where F_{ij} is the rate of toxicant ingestion (mg day^{-1}) by animal group i preying on food item j and C_o^j is the toxicant concentration in food item j. Ingested toxicant may then either be assimilated into the animal's tissues or eliminated from the animal's body. Toxicant assimilation is modeling using an empirical efficiency factor representing the fraction of ingested toxicant which is assimilated. The toxicant assimilation rate for animal group i then becomes:

$$\begin{aligned} J_a^i &= \sum_j \alpha_{ij} F_{ij} \\ &= U_T^i \sum_j \alpha_{ij} \beta_j^i C_o^j \sum_h p^i_{j|h} p_h^{ij} \qquad (3\text{-}207) \end{aligned}$$

where α_{ij} is the assimilation efficiency factor when animal group i eats food item j. The terms α^{ij} must be greater than or equal to 0.0 but less than or equal to 1.0.

Metabolic degradation of toxicant within organisms is modeled as a first-order decay process:

$$J_d^i = K_{met}^i \left(C_o^i M_o^i\right) \qquad (3\text{-}208)$$

where K_{met}^i is a first order rate constant for degradation of toxicant in animal group i. The predation loss term accounts for the removal of pesticide mass when other animals prey on and ingest toxicant mass from animal group i:

$$J_p^i = C_o^i \sum_j \beta_i^j U_T^j \sum_h p_{i|h}^j p_h^{ij} \qquad (3\text{-}209)$$

Substituting the above rate expressions into the overall toxicant mass balance equation for animal group i,

$$\frac{d\left(M_o^i C_o^i\right)}{dt} = U_T^i \sum_j \alpha_{ij} \beta_j^i C_o^j \sum_h p_{j|h}^i p_h^{ij}$$
$$- K_{met}^i \left(C_o^i M_o^i\right) - C_o^i \sum_j \beta_i^j U_T^j \sum_h p_{i|h}^j p_h^{ij} \qquad (3\text{-}210)$$

Organisms are modeled as subgroups, or populations depending upon the level of detail required in simulating animal movement. Animals modeled as subgroups will move randomly en masse between locations as determined by the Markov transition matrix; animals modeled as populations will be distributed among locations based on the product of initial population distributions and the transition matrix. The toxicant mass balance equation is then written for each subgroup and population, resulting in a system of first order differential equations for the entire food chain. Movement probabilities (p_h^{ij}) are computed by the animal movement model, and a fourth-order Runge-Kutta integration scheme is used to solve the system of mass balance equations (Equation 3-210) for the mass of toxicant $(M_o^i C_o^i)$ in each subgroup or population at the end of each daily time step.

The biomass of individuals and populations is assumed to be constant. Ultimately, a population model can be incorporated and the estimates of M_o^i at each time step would be an output of that model. The assimilation efficiency factors α_{ij} can hopefully be derived from thermodynamic considerations or from empirical approaches such as proposed by Jorgensen (1984). They are typically considered to be functions of the lipophilicity of the compound, fat content and metabolic rate of the predator, and the size of the particle or interaction of the chemical with the prey ingested (Tinsley 1979). The assimilation efficiency is also a function of the uptake route (i.e., ingestion versus inhalation).

Some food items or items ingested during the process of obtaining food can be handled as special cases of Equation (3-206). For instance, soil ingestion does not require a "capture probability" and only depends upon the product of the soil ingestion rate, the concentration of the soil in habitat "h", and the probability of being in habitat "h". Uptake by inhalation takes on a similar form. Uptake in ingested water depends on the presence of ponded water in addition to the factors listed above. Direct ingestion of pesticide may also occur if the chemical is deposited in the form of granules.

The U_T^i for the food items of soil animals at the base of the food chain may be difficult to define individually. These animals (earthworms, arthropods, etc.) move between soil horizons and are exposed to pesticides in soil, water, and ingested detritus. The toxicant mass balance equations for these organisms are therefore formulated differently than for the higher-order animals:

$$\frac{d(C_oM_o)^i}{dt} = k_TC_TV_T - K_{met}(C_oM_o)^i - J_p^i \qquad (3\text{-}211)$$

In this model all of the feeding forms are lumped into a single mass-transfer coefficient, k_T, which describes the net uptake of pesticides (C_TV_T) from the soil. C_T is the total pesticide concentration on a total-volume basis and V_T is the total volume of the soil compartment.

In order for the modeled concentrations in soil animals to approach observed values in the literature, the values of k_T and K_{met} must be carefully selected. This is done in the model by making use of a terrestrial bioconcentration factor, defined as the ratio of concentration in the biomass (C_o) to the concentration the soil (C_s):

$$BCF = \frac{C_o}{C_s} \qquad (3\text{-}212)$$

This ratio can be related to the coefficients K_{met} and k_T. If we assume that the predation loss term J_p^i of the organisms is small compared to the biomass M_o, and that M_o is relatively constant, then Equation (3-211) can be rewritten as

$$\frac{dC_o}{dt} = \frac{k_TC_TV_T}{M_o} - K_{met}C_o \qquad (3\text{-}213)$$

The quantity C_T can be expressed as a function of C_s by making use of the soil chemical mass balance equation:

$$C_T = (\rho_s + \frac{\Theta}{K_d})\ C_s \qquad (3\text{-}214)$$

where ρ_s is the soil bulk density, θ is the soil water content, and K_d is the partition coefficient.

Equation (3-212) can then be written as:

$$\frac{dC_o}{dt} = \frac{k_TV_T(\rho_s + \frac{\Theta}{K_d})\ C_s}{M_o} - K_{met}C_o \qquad (3\text{-}215)$$

At steady state, $\frac{dC_o}{dt} \rightarrow 0$, and therefore

$$k_T V_T \frac{(\rho_s + \frac{\theta}{K_d})\, C_s}{M_o} = K_{met}\, C_o \qquad (3\text{-}216)$$

Solving for the soil animal mass transfer coefficient:

$$k_T = \frac{M_o K_{met} C_o}{V_T(\rho_s + \frac{\theta}{K_d})C_s} \qquad (3\text{-}217)$$

At steady state the ratio C_o/C_s is equal to the bioconcentration factor BCF. V_T can be expressed as $A\,\Delta Z$ where A is habitat area and ΔZ is soil compartment depth. The term M_o/A is defined as the organism density, ρ_o. Substituting these relationships into Equation (3-217):

$$k_T = \frac{\rho_o BCF}{K_{met} \Delta Z(\rho_s + \frac{\theta}{K_d})} \qquad (3\text{-}218)$$

As long as BCF and K_{met} are reasonably well known, k_T can be defined from Equation (3-218) so that soil animals attain a concentration of approximately (C_sBCF) at steady state. This approach to parameter estimation is similar to that described in Donigian and Dean (1985). Review of the literature on uptake and metabolism of chemicals by earthworms presented in Roberts and Dorough (1985) indicates that in general data are available to estimate coefficients in this way.

3.6 THE MONTE CARLO MODULE (MC)

This section describes the Monte Carlo method used for uncertainty analysis of the TEEAM model. Given a set of deterministic values for each of the input parameters, $X_1, X_2 \ldots X_n$, the TEEAM model computes a number of soil, animal, and plant output parameters Y_i:

$$Y_i = g\,(X_1, X_2, X_3 \ldots X_n) \qquad (3\text{-}219)$$

Application of the Monte Carlo simulation procedure requires that at least one of the input variables, $X_1 \ldots X_n$, be uncertain with the uncertainty represented by a cumulative probability distribution. The method involves the repeated generation of pseudo-random number values of the uncertain input variable(s) (drawn from known distributions and within the range of any imposed bounds) and the application of the model using these values to generate a series of model responses, i.e., values of Y_i. These responses are then statistically analyzed to yield the cumulative probability distribution of the model response. Thus, the various steps involved in the application of the Monte Carlo simulation technique involve:

1) Selection of representative cumulative probability distribution functions for describing uncertainty in the relevant input variables.

2) Generation of pseudo-random numbers from the distributions selected in (1). These values represent a possible set of values for the input variables.

3) Application of the model to compute the derived output(s).

4) Repeated application of steps (2) and (3) to produce a sufficiently large sample of model outputs for frequency analysis.

5) Presentation of the series of output (random) values generated in step (3) as a cumulative probability distribution function (CDF).

6) Analysis and application of the cumulative probability distribution of the output as a tool for decision making.

The input variables required by TEEAM can be broadly classified into two different sets that exhibit different uncertainty characteristics. These are:

- Variables that describe the chemical, biochemical, and toxicological properties of the chemical of concern. Examples of these variables include the octanol-water partition coefficient, acid, neutral, and base catalysed hydrolysis rate, soil-adsorption coefficient, Henry's Law Constant, etc.

- Variables that describe the environmental properties of the various media and impact the fate and transport of the pollutant within each medium. Examples of these variables include the soil porosity, organic carbon content, metabolic degradation rates, etc.

Uncertainty in the first set of variables primarily arises due to laboratory measurement errors or theoretical methods used to estimate the numerical values. In addition to experimental precision and accuracy, errors may arise due to extrapolations from controlled (laboratory) measurement conditions to uncontrolled environmental (field) conditions. Further, for some variables semi-empirical methods are used to estimate the values. In these cases, errors in using the empirical relationships also contribute to errors/uncertainty in the model outputs.

Uncertainty in the second set of variables may include both measurement and extrapolation errors. However, the dominant source of uncertainty in these is inherent natural (spatial and temporal) variability. This variability can be interpreted as site-specific or within-site variation in the event that the model is used to analyze exposure due to the use of a toxicant at a particular site. Alternatively, it can represent a larger scale (regional/national) uncertainty if the model is used to conduct exposure analysis for a specific chemical or ecosystem on a generic, nationwide or regional basis. Note that the distributional properties of the variables may change significantly depending upon the nature of the application.

Whatever the source of uncertainty, the Monte Carlo method requires that the uncertainty in input parameters be quantified by the user. This implies that for each input parameter deemed to be uncertain, the user select a distribution and specify the parameters that describe the distribution. The following sections describe the methods by which the TEEAM Monte Carlo module generates random numbers and analyzes model outputs.

3.6.1 Description of Monte Carlo Parameter Distributions

The Monte Carlo Module has the ability to generate data from a number of probability distributions, including uniform, normal, log-normal, exponential, and Johnson SB. A description of each of these distributions is provided in the following paragraphs, including parameters of the distributions, equations for the probability and cumulative density functions, and a brief discussion of the properties of each distribution.

Uniform Distribution--

A uniform distribution is a symmetrical probability distribution in which all values within a given range have an equal chance of occurrence. A uniform distribution is completely described by two parameters: 1) the minimum value (lower bound) A, and 2) the maximum value (upper bound) B. The equation for the uniform probability density distribution of variable x is given by:

$$f_u(x) = \frac{1}{(B - A)} \qquad (3\text{-}220)$$

where f(x) is the value of the probability density function for x. The cumulative distribution F(x) is obtained by integrating Equation (3-220). This yields the probability distribution:

$$F_u(x) = \frac{(x - A)}{(B - A)} \qquad (3\text{-}221)$$

where $F_u(x)$ is the probability that a value less than or equal to x will occur.

Normal Distribution--

The normal distribution refers to the well known bell-shaped probability density function. Normal distributions are symmetrical about the mean value and are unbounded, although values further from the mean occur less frequently. The spread of the distribution is generally described by the standard deviation. The normal distribution has only two parameters: the mean and the standard deviation. The probability density function of x is given by:

$$f_n(x) = \frac{1}{S_x\sqrt{2\pi}} \exp\left[-0.5\left(\frac{x - m_x}{S_x}\right)^2\right] \tag{3-222}$$

where S_x is the standard deviation, and m_x is the mean of x. The cumulative distribution is the integral of the probability density function:

$$F_n(x) = \int_{-\infty}^{x} f_n(x)dx \tag{3-223}$$

The above integration must be performed numerically, but tables of numerically-integrated values of $F_n(x)$ are widely available in the statistical literature.

Log-Normal Distribution--

The log-normal distribution is a skewed distribution in which the natural log of variable x is normally distributed. Thus, if y is the natural log of x, then the probability distribution of y is normal with mean m_y, and standard deviation S_y and a probability density function similar to Equation (3-222). The mean and standard deviation of x (m_x and S_x) are related to the log-normal parameters m_y and S_y as follows:

$$m_x = \exp[m_y + 0.5(S_y)^2] \tag{3-224}$$

$$S_x^2 = m_x^2[\exp(S_y^2) - 1] \tag{3-225}$$

To preserve the observed mean and standard deviation of x, the parameters of the log-normal distribution (m_y and S_y) are therefore selected such that the above relationships are satisfied. Note that m_y and S_y do not equal the natural logs of m_x and S_x respectively. Log-normal distributions have a lower bound of 0.0 and no upper bound, and are often used to describe positive data with skewed observed probability distributions.

Exponential Distribution--

The probability density function for an exponential distribution is described by an exponential equation:

$$f_e(x) = \frac{\exp(-x/m_x)}{m_x} \tag{3-226}$$

where m_x is the mean of x. The cumulative distribution is given by:

$$F_e(x) = 1 - \exp(-x/m_x) \tag{3-227}$$

The exponential distribution is bounded by zero; the probability density function peaks at zero and decreases exponentially as x increases in magnitude.

The Johnson System of Distributions--

The Johnson system involves two main distribution types: SB (Log-ratio or bounded) and SU (unbounded or hyperbolic arcsine). These two distribution types basically represent two different transformations applied to the random variable such that the transformed variable is normally distributed. The specific transformations are:

$$\text{SB:} \quad Y = \ell n\left(\frac{(x-A)}{(B-x)}\right) \tag{3-228}$$

$$\text{SU:} \quad Y = \ell n\left[\frac{x-A}{B-x} + \left(1 + \left(\frac{x-A}{B-x}\right)^2\right)^{0.5}\right] \tag{3-229}$$

where:

ℓn = natural logarithm transformation
x = untransformed variable with limits of variation from A to B.
Y = the transformed variable with a normal distribution

Selection of a particular Johnson distribution for sample data set is accomplished by plotting the skewness and kurtosis of the sample data. The location of the sample point indicates the distribution for the sample data.

For additional details of the Johnson system of distributions, the reader is referred to McGrath et al. (1973) and Johnson and Kotz (1970).

3.6.2 Uncertainty in Correlated Variables

In many cases model input variables are correlated due to various physical mechanisms. Monte Carlo simulation of such variables requires not only that parameters be generated from the appropriate univariate distributions, but also that the appropriate correlations be preserved in the generated input sequences. The Monte Carlo module currently has the ability to generate correlated normal and log-normal numbers. The procedures used are described in the following paragraphs.

The correlation coefficient is a measure of the linear dependence between two random variables and is defined as:

$$\rho_{x,y} = \frac{\mathrm{cov}(x,y)}{\sigma_x \sigma_y} \qquad (3\text{-}230)$$

where:

$\rho_{x,y}$ = the correlation coefficient between random variables x any y
$\mathrm{cov}(x,y)$ = the covariance of x and y as defined below
σ_x, σ_y = the standard deviation for x and y.

The covariance of x and y is defined as:

$$\begin{aligned} \mathrm{cov}(x,y) &= E[(x-m_x)(y-m_y)] \\ &= \int_{-\infty}^{+\infty}\!\!\int (x-m_x)\,(y-m_y)\, f_{x,y}(x,y)\, dxdy \end{aligned} \qquad (3\text{-}231)$$

where

E = the expected value
m_x, m_y = the mean of the random variables x and y
$f_{x,y}(x,y)$ = the joint probability distribution of x and y.

Note that the linear correlation coefficient between x and y can be computed using

$$\rho_{x,y} = \frac{\sum_{i=1}^{n} x_i y_i - n\, m_x m_y}{\left(\sum_{i=1}^{n} (x_i^2 - nm_x^{-2}) \left(\sum_{i=1}^{n} (y_i^2 - nm_y^{-2}) \right) \right)^{0.5}} \qquad (3\text{-}232)$$

To generate correlated random variables three steps are required. First uncorrelated normally distributed random numbers are generated. This vector is then transformed to a vector of normally distributed numbers with the desired correlation. Finally, the normally distributed numbers are transformed to numbers with the desired distribution.

The transformation of uncorrelated to correlated normal numbers consists of multiplying the uncorrelated vector of numbers with a matrix B:

$$Y' = B\, e \qquad (3\text{-}233)$$

where

e = the vector of uncorrelated, normally distributed random numbers
B = an N by N matrix

Y' = a vector of standard normal deviates of mean zero and standard deviation of unity

The matrix B is related to the variance-covariance matrix S as follows:

$$S = BB^T \tag{3-234}$$

where B^T is the transpose of the matrix B. Since the normal variables Y' have means of zero and unit variances, the variance-covariance matrix is equivalent to the correlation matrix.

Thus, if the correlation matrix S is known, B can be found from Equation (3-234) by using a Cholesky decomposition algorithm. This algorithm will decompose a symmetric positive definite matrix, such as S, into a triangular matrix such as B.

Having generated a vector of correlated normally distributed random numbers, the vector Y' can be converted, through appropriate transformations, to the distribution of choice. Thus for parameters X_i that have a normal distribution, the Y' numbers are transformed as follows:

$$X_i = m_x + \sigma_x(Y_i') \tag{3-235}$$

For parameters that follow the lognormal distribution, the following transformation applies:

$$X_i = \exp[(Y_i')\ (\sigma_{\ln,i}) + \mu_{\ln,i}] \tag{3-236}$$

where

$\mu_{\ln,i}$ is the log mean of the i^{th} parameter. (3-237)

$\sigma_{\ln,i}$ is the log standard deviation of the i^{th} parameter (3-238)

Other distributions can be easily incorporated into the analyses at a later time when suitable transformations from the normal distribution can be found. It is important to note that in using this technique, the correlations are estimated in normal space so if these correlations are estimated using actual data, the data should be transformed to a normal distribution before correlation coefficients are estimated.

For two correlated variables, one with a normal distribution (x_2) and the other with a log normal distribution (x_1), the following equation is used to transform correlations to normal space (Mejia et al. 1974):

$$\rho_{y_1,y_2} = \frac{\rho_{x_1,x_2}\ [\exp(\sigma_{y_1}^2) - 1]^{\frac{1}{2}}}{\sigma_{y_1}} \tag{3-239}$$

where

ρ_{y_1,y_2} = the correlation coefficient between the two variables in the normal space

ρ_{x_1,x_2} = the correlation coefficient between the two variables in the arithmetic space

σ_{y_1} = the variance of y_1 derived from Equation (3-224)

If both x_1 and x_2 are log-normally distribution then the correlation coefficient in the normal space is transformed using Mejia et al (1974):

$$\rho_{y_1,y_2} = \frac{1}{S_{y_1} S_{y_2}} \ln\{1 + \rho_{x_1,x_2} \left| \frac{S_{x_1} S_{x_2}}{m_{x_1} m_{x_2}} \right|\} \qquad (3\text{-}240)$$

where the relationships between S_{x_1} (S_{x_2}) and S_{y_1} (S_{y_2}) are given by Equations (3-224) and (3-225).

3.6.3 Generation of Random Numbers

Having selected the distribution for the various input parameters, the next step is the generation of random values of these parameters. This requires the use of pseudo-random number generating algorithms for Normal and Uniform numbers. There exist numerous proprietary as well as non-proprietary subroutines that can be used to generate random numbers. A number of these are comparable in terms of their computational efficiency, accuracy, and precision. The routines included in TEEAM have been checked to ensure that they accurately reproduce the parameters of the distributions that are being sampled.

SECTION 4

MODEL INSTALLATION AND EXECUTION

This section describes how to load the TEEAM software into an IBM-PC compatible computer from the supplied floppy disks, how to verify that the software has been loaded properly, and how to execute TEEAM simulations. The hardware and software required for installing TEEAM on an IBM-PC computer are also discussed. If a computer other than an IBM-PC compatible is to be used, some INCLUDE files will have to be modified and the software will have to be recompiled.

4.1 IBM-PC COMPATIBLE ENVIRONMENT REQUIREMENTS

4.1.1 Hardware

An IBM-PC compatible computer with 640K memory, one floppy disk drive, and at least 5 megabytes of available hard disk storage is the minimum hardware requirement. The floppy disk drive is necessary to download the software and test data files as supplied. Either a 360 KByte (DSDD) drive or a 1.2 MByte (DSHD) drive can be used; the installation floppy disks can be sent in either format. A math coprocessor (8087, 80287, or 80387) must also be present.

4.1.2 Software

The TEEAM software was developed using an MSDOS 3.2 operating system. Earlier versions of PCDOS or MSDOS which are able to recognize file directories should also be compatible.

The DOS supplied ANSI.SYS driver must also be available. This driver is installed by modifying the DOS specific CONFIG.SYS file (located in the root directory) to contain the following line:

```
DEVICE = <path> ANSI.SYS
```

where <path> is the location (directory) of the ANSI.SYS file. This file will normally be located in a directory containing other DOS specific files; the location of this file (or even its presence) was determined by the individual who originally configured the microcomputer. If this file is not available, it will be necessary to consult with an individual who is familiar with the MSDOS operating system to determine the steps necessary to have it available for the TEEAM software.

The CONFIG.SYS file may also have to be modified to specify how many files are available to the TEEAM software. It the statement 'FILES =' is not present or it is present but with a value less than 20 (e.g., 'FILES = 10') then the statement 'FILES = 20' (without the quote marks) should be added to the CONFIG.SYS file.

If the installation disks are 360K format, it will be necessary to have the DOS Restore command available.

4.2 LOADING EXECUTABLE CODES AND TEST DATA FILES

The executable code and test data files can be loaded onto the hard disk of the target computer by taking the following steps:

1. Insure that the target hard disk does not have a directory called TEEAM and that the hard disk is in the root directory.

2. Put the TEEAM floppy disk labeled 'MASTER' in the floppy disk drive.

3. Make the floppy disk drive the default drive (e.g., type 'A:' if the floppy drive is the A drive).

4. Type INSTALL <d1> <d2>, where <d1> is the source drive (e.g., A) and <d2> is the target drive (e.g., C). The spaces between the INSTALL command and the drive designators are required; colons should not be present in the drive designators.

5. If additional disks are required, you will be prompted to insert them in the floppy drive and press return.

6. After the executable code and test data files have been loaded, you will be asked if you want to load the TEEAM source code. The source code is only necessary if you wish to make modifications to the code and it is not necessary to load these files (and thus, decrease the available storage on your hard disk) if you do not want to make modifications. The source code can always be obtained from the floppy disks if you require it at a future date.

Using the INSTALL batch file is a convenience but is not necessary if you wish to copy the TEEAM files within your own directory structure. The INSTALL file creates a subdirectory (called TEEAM) on the hard disk, copies the executable code, some batch files, and run files into this directory, creates several subdirectories within the directory TEEAM and copies the test data files into these directories, and, optionally creates a subdirectory of the source code and include files.

4.2.1 Executing Test Data Inputs

A batch file is supplied which will execute all of the test data files provided, one after another. This file, TESTRUN.BAT is available within the TEEAM subdirectory and can be executed by typing TESTRUN while within the TEEAM subdirectory.

These test data sets can be executed individually, if desired, by: (1) copying the appropriate test run file (labeled TESTDAT.n, where n = 1 to the number of test data sets) to the file name TMRUN.DAT, (2) erasing the file KECHO.PRN if present, and (3) then typing TEEAM (followed by a return) to start execution.

4.2.2 Verifying Test Data Outputs

Running the batch file TESTRUN.BAT will create output files with the extension .PRN within the test data set subdirectories (labeled TESTDAT.n, where n = 1 to the number of test data sets). Within these subdirectories will be files with the same prefix but with the extension .VRF. Each of the .PRN files should be compared to the corresponding .VRF file either by using an editor to visually compare the results or by using the DOS compare utilities FC (DOS 3.2 or greater) or COMP (earlier versions of DOS).

4.3 GENERAL PROCEDURES FOR TEEAM EXECUTION

This section contains descriptions of techniques and suggestions for normal (operational) execution of TEEAM. It is generally convenient to locate all of the input files pertaining to a specific problem within their own subdirectory. The input files should be developed using the file descriptions of Section 5. It will normally be useful to start with the test input data files provided and edit them to meet the specifications of the problem at hand.

The names chosen for the input files should be specific to the problem to reduce the potential for confusing these files with those developed for alternate problems - TEEAM enforces no restrictions on the names chosen, either for the prefix or extension (DOS limits the prefix to 8 characters and the extension to 3 characters). It is good practice to choose an extension which implies an input file (e.g., .IN or .DAT) or output file (e.g., .OUT or .PRN). The names of the files used and the path describing where the files are located (the subdirectory) are defined in the file TMRUN.DAT, the run control file (see Section 5.2.1). The file TMRUN.DAT must be in the TEEAM subdirectory. When all of the necessary files are complete, TEEAM can be executed by typing TEEAM followed by a return.

The PATH statement in the TMRUN.DAT file can be used to specify the directories or subdirectories where the model input and output files are located. When the PATH statement is used in the TMRUN.DAT file, the defined path must end with the backslash character ('\'). The defined path will pertain to all files which are defined after that path statement until another path is defined.

If the file subdirectory is a subdirectory within the TEEAM subdirectory, the path defined should not begin with a backslash. If the file subdirectory is external to the TEEAM subdirectory, the defined path should begin with a backslash (this implies to DOS that the search for the subdirectory should begin from the root directory).

The path record can also be used to define files which are located on different drives. This is potentially useful to increase the execution speed of multiple habitat and Monte Carlo simulations. Both multiple habitat and Monte Carlo simulations use scratch (unformatted) files for temporary storage of data and these scratch files are opened with the last defined path (note that a PATH record can be the last record of the file records within TMRUN.DAT). If the last path indicates that the files are to be located on a RAM disk (please consult your DOS manuals for defining a RAM disk) execution speed will be measureably increased.

4.4 MACHINE AND COMPILER DEPENDENCIES

The code has been designed to be implementation independent where an implementation would include computer make and type, input/output devices used, and brand and version of FORTRAN 77 compiler used. The model is compatible with the DEC VAX running VMS, PRIME 50 series running PRIMOS, IBM hardware or compatible mainframes running OS/VS2 MVS, and IBM PC compatibles running MS DOS. Minimal knowledge of the particular operating system is required of the user.

There are a few exceptions to the rule of implementation independence which were necessary to provide useful features for the user interface and to follow EPA recommendations for FORTRAN code development. Extensive use has been made of INCLUDE files for defining COMMON variables and PARAMETERs (see Section 9). The use of INCLUDE files ensures that variables and parameters common to all subroutines will be of the same size and type;

unfortunately, the format for INCLUDE statements is dependent on the FORTRAN compiler used. Currently, the only "work-around" for this compiler dependence is to provide versions of the code for alternate compilers.

An additional compiler-dependency is the definition of the minimum and maximum values of single precision real numbers which do not result in underflows and overflows. These values are defined in a single INCLUDE file and are provided to prevent "system crashes" or unintelligible system error messages; these values are used to check the intermediate calculation of variables and supply a warning to the user if an underflow or overflow condition exists and to provide an organized exit from the software if the condition is fatal. Since these values are located in a single file, it is a relatively simple matter to change the values provided to values which would be more appropriate to the FORTRAN compiler being used.

A screen management routine has been supplied to present the software in operation. If it is defined that an IBM PC (or compatible) computer is being used, the screen will be updated without scrolling text off the top of the screen. If this IBM PC option is not set (in the same INCLUDE file as above) before compiling, TEEAM execution information will be listed line-by-line to the standard output device.

SECTION 5

INPUT SEQUENCE DEVELOPMENT

5.1 OVERVIEW OF TEEAM INPUT DATA

This section describes the contents and formats of the various data files required to run TEEAM. In general, all input to the model occurs sequentially from batch files. These files may be created or edited from sample input files which are supplied with the code using a text editor on the user's computer system. A separate batch input file is required for each of the following TEEAM modules if they are used in the simulation:

- Execution Supervisor (EXESUP)
- Aerial Spray (FSCBG)
- Spray Grid Definition (GRDDEF)
- Terrestrial Fate and Transport (TFAT)
- Plant Growth and Translocation (PLTGRN and PLTRNS)
- Terrestrial Animal Exposure (APUM)
- Monte Carlo (MC)

The Execution Supervisor data file selects the modules to be executed, defines the names of the input files to be utilized, and is required for all TEEAM runs. The TFAT module data file defines the physical and transport properties for each habitat and is also required for all TEEAM runs. The remaining modules (and their corresponding batch input files) may or may not be used depending upon options selected in the Execution Supervisor file. The modules FSCBG and GRDDEF compute the distribution of pesticide applied during spray events. The plant growth and translocation modules compute the growth of plants and the transport of pesticides through the plant roots and aboveground biomass. The APUM module calculates the uptake and assimilation of pesticide by animals ingesting water, pesticide granules, soil, plants, and other animals or inhaling contaminated air. Finally, the Monte Carlo module generates random inputs to the various modules for Monte Carlo runs of TEEAM; inputs for this module describe the probability distributions of various model parameters. Note that Monte Carlo simulations can only be performed for one habitat simulation.

Specific formats for each module and corresponding input file are described in Section 5.2 and in Tables 5.1 through 5.9. Due to the length of these tables, they are presented collectively at the end of this section. In the format descriptions each data line is referred to as a "Record." These records may consist of one line of data or may be repeated as necessary (i.e., for each soil horizon, animal, or crop). Records are labeled for reference by the appropriate module acronym followed by a sequential number. For instance, the first data record in the TFAT module is labeled "TFAT1." Record descriptions in Tables 5.1 through 5.9 consist of one line listing the record number and the names of the input variables contained in the record, one line describing the required FORTRAN input format, and several lines defining the input variables and their appropriate units.

Note that since several of the modules were developed from pre-existing model codes, data input formats vary significantly from module to module. TEEAM data records are usually formatted, meaning that each input variable on a record occupies a field of specified length. For instance, the format (2F10.0) indicates that there are two data fields of length 10 each. Character formats are also used extensively to read labels and option flags. For example, the format (A20) indicates that a character string up to 20 characters long (including blanks) is read. All character strings read by the model are converted to upper case letters immediately after input; the model therefore does not differentiate between upper case and lower case labels and responses.

A feature common to all TEEAM input files except for the FSCBG module is the Comment line. Comment lines may be inserted anywhere in the input data files, and are indicated by the presence of three asterisks ("***") as the first non-blank characters in the line. These lines are ignored by the model for computational purposes and allow the user to type in comments, table headings, and other information useful in making the input file more understandable.

5.2 DESCRIPTION OF INPUT FILES FOR TEEAM MODULES

5.2.1 Execution Supervisor

The run control file which is the input to the execution supervisor is the only input file which cannot have an optional name; it must be named "TMRUN.DAT" and it must be located within the default directory. This file is used to define which options (modules) are selected for a simulation and what the files are to be named that are used for input and output. Additionally, several parameters which are required for simulation control, such as starting and ending dates, are also defined by this file. Figure 5.1 illustrates a sample TMRUN.DAT file.

There are three major groups of input data: 1) options, 2) files, and 3) global parameters. Formats for these data are shown in Table 5.1. The simulation trace level can also be defined with this file. The simulation trace level is used to display to the screen which subroutine TEEAM is in during execution.

All of the potential options have default values and, if an option is not specifically set, the default value will be assumed. These defaults are as follows: TFAT=ON, AERIAL SPRAY=OFF, FSCBG=OFF, PLTGRN=ON, APUM=ON, MONTE

```
*** Sample TMRUN.DAT file
***
*** Options
TFAT                           ON
PLTGRN                         ON
AERIAL SPRAY                   OFF
FSCBG                          OFF
APUM                           ON
NHAB                           1
MONTE CARLO                    OFF
ENDRUN
*** Files
PATH                           \EPAB7\mcnew\DATA\
METEROLOGY                     MET.SML
FSCBG OUTPUT                   CBGF00
FSCBG INPUT                    @FSDATA\KFSPR.IN
PLTGRN                         KPLNT.dat
APUMIN                         NOCUTWRM.IN
GRID DEFINITION                GRDDEF1.IN
MCIN                           @RANDU.IN
TFAT                           PRZM.ONE
*** separate path for output files for convienience
PATH                           \EPAB7\MCNEW\
APUMOUT                        NOCUTWRM.PRN
ANIMAL TIME SERIES             KRSLTS.PRN
CONCENTRATIONS                 KCONC.PRN
HYDROLOGY                      KHYDRO.PRN
PESTICIDES                     kflps.prn
TIME SERIES                    KFLTS.PRN
MCOUT                          MCOUT.PRN
MCOUT2                         MCOUT2.PRN
ENDFILES
***  Global data
  010450             300450
     .75    0.000        2     36.2
*** Daylight hours for Tifton GA
     10.2     10.9     11.9     12.8     13.7     14.0
     13.9     13.5     12.2     11.2     10.4     10.0
TRACE                     0
```

Figure 5-1. Sample Execution supervisor input data file (TMRUN.DAT)

CARLO=OFF, and NHAB=1. The options section must end with ANAME="ENDRUN" (Table 5.1) even if all of the default values are to be used.

Note that turning PLTGRN "ON" invokes both the EPIC plant growth algorithm and the plant transportation module PLTRNS. If PLTGRN is "OFF," plant growth is not shut off; rather the plant growth algorithm in the original version of PRZM is enabled.

The file records of the execution supervisor input are used to assign the user supplied names and locations of the files required for a simulation to the appropriate TEEAM file. If files are defined within these records which are not necessary because of the options selected in the options records (EXESUP1), the file name is ignored.

The global parameters records are used to define certain environmental and simulation control parameters which need to be defined for all habitats and thus are not specific to each TFAT habitat.

The trace level record is, in general, only necessary for debugging problems with a simulation. If the trace level is set to a value greater than one, the subroutine that TEEAM is currently executing during a simulation, as well as the path of subroutine calls to access that subroutine, are displayed on the standard output device. A trace can be useful for debugging a simulation but, when used, can increase execution time considerably. If the trace level record is not included in the EXESUP data set, a default value of 3 will be assumed. A value of 3 indicates that subroutine calls three levels deep will be displayed.

5.2.2 Input Data for the FSCBG Module

The FSCBG module was adapted from the FSCBG code (Dumbauld, Bjorklund, and Saterlie 1980) for incorporation into the TEEAM model. The purpose of the FSCBG module is to calculate the top-of-canopy deposition resulting from an aerial or ground spray event. The input format for the FSCBG module (Table 5.2a) is similar to the original input requirements described in Dumbauld, Bjorklund, and Saterlie (1980). Comment lines cannot currently be utilized in the FSCBG input file.

Only the first record, the simulation title, uses a FORTRAN format. All of the other records use list directed input formatting. In list directed formatting, data values are entered on a line in columns 1 to 80. All data values are separated by a single comma (,). If a data value is intended to be omitted, a comma should be entered immediately after the preceding comma. A slash (/) may be used to indicate an end of line. If a slash is entered before all data values have been supplied, the remaining variables on that line are left unitialized.

The second record required by the FSCBG module is an array of option integers (ISW). The values which these integers can have and the resulting actions taken are presented in Table 5.2b. Most of the options present in the original FSCBG code have been deleted for the TEEAM installation. As a result of this, the option numbers appearing in Table 5.2b are no longer sequential but the options still available correspond to the original FSCBG numbering system.

5.2.3 Input Data for the Spray Grid Definition Module

The spray grid definition module uses the output from the FSCBG aerial spray application module and computes the average top-of-canopy deposition to each habitat. To accomplish this task, the spray grid definition module has to be given the correspondence between the FSCBG receptor grid (the spatial coordinate system defining the area which could potentially receive a spray application or drift from a spray application) and the individual habitats. Given this information the spray grid definition module is able to calculate the average top-of-canopy depositions.

The input file to the spray grid definition module defines three types of data: 1) the location of habitats with respect to the aerial spray grid (FSCBG receptor grid), 2) the number and dates of spray events, and 3) parameters defining how the top-of-canopy data (FSCBG output) should be distributed to soil and foliage and within the plant canopy. These data are defined in Table 5.3.

The locations of habitats and the definition of the FSCBG receptor grid are described by Records GRID1-GRID4. This module will generate the FSCBG receptor grid based on the number of east-west and north-south grid points selected in Record GRID2, the initial x- and y-coordinates, and increments for x- and y-coordinates, (GDX and GDY, respectively) in Records GRID3 and GRID4. Note that each grid point generated represents the center of a subgrid area of dimensions GDX by GDY. These grid points are the locations where FSCBG computes the top of canopy pesticide deposition for each subgrid area.

The locations of habitats are defined by entering the x- and y-coordinates of the southwest and northeast corners of each habitat on Record GRID1. These coordinates should be within the FSCBG receptor grid. It is preferable, but not necessary, that the habitat corner coordinates be specified as the midpoint between receptor grid coordinates. If the midpoints are used, the habitat area computed based on the coordinates will be the same as the area computed by summing all the subgrid areas within a habitat.

The data on number and dates of spray events and the parameters defining how the FSCBG output should be distributed within the plant canopy are passed on to the TEEAM execution supervisor for processing by the TFAT module.

5.2.4 Input Data for the Terrestrial Fate and Transport Module (TFAT)

The Terrestrial Fate and Transport Module (TFAT) uses two input data files: a meteorological data file and a parameter file. The meteorological data file contains daily values of precipitation, potential evapotranspiration, temperature, solar radiation, and wind speed. Formats for this file are described in Table 5.4. The parameter file contains the following four groups of data for each habitat describing the transport of pesticide:

• Hydrology and Crop Data	(Records TFAT1 - TFAT11)
• Pesticide Application Data	(Records TFAT12 - TFAT19)
• Soils Data	(Records TFAT20 - TFAT27A)
• Output Specification	(Records TFAT28 - TFAT30)

Specific formats for each parameter data group are shown in Table 5.5 and are discussed below. Note that the entire parameter data set for the TFAT module should be repeated as a set for each habitat.

The hydrology and crop data group consists of data describing the runoff, erosion, infiltration, and crop conditions at the soil surface. Record TFAT1 is a title used to identify input and output files for the TFAT run, while Record TFAT2 is a title for the hydrology data group. Record TFAT3 contains data describing initial crop conditions, the area of the habitat, and the number of time steps used by the ponding and infiltration algorithms. Note that if the FSCBG and GRDDEF modules are used, the area of the field entered here should be the same as the area defined by the the GRDDEF habitat spray grid coordinates. Record TFAT4 consists of data required by the ponding and infiltration routines, including Green-Ampt parameters and initial conditions. Records TFAT6 and TFAT7 contain surface erosion parameters; note that TFAT7 is not required if erosion is not simulated (ERFLAG = 0 on TFAT6). Finally, Records TFAT8 through TFAT11 describe the growth and runoff properties of the various crops which are simulated.

The pesticide application data group (Records TFAT12-TFAT19) consists of data describing the timing, amount, and distribution of TFAT pesticide applications. These data are used to define application events (e.g., granular, direct to soil or soil incorporation) for which off-site drift is not an issue. Note that additional applications may also occur as calculated by the FSCBG module. If a spray event in FSCBG is specified on the same day as an application event in TFAT, the spray application event parameters will override the TFAT parameters. Also included in this data group are several pesticide volatilization parameters. Record TFAT12 is a 1 to 80 character title for the pesticide application data group. Record TFAT13 contains the number of pesticide applications to be described in Record TFAT14. Record TFAT14 is repeated for each application and contains the date of application, the amount, the depth of incorporation, and for granular applications, concentration of pesticide in granules. The type of application is selected by the parameters FAM and KANOPT on Record TFAT15, and the remaining input of application data depends upon the values of these parameters. If FAM=1, the application is incorporated into the soil and no further application data except Records TFAT18 and 19 are required. If FAM = 2 or 3, pesticide is applied to the plant foliage. FAM = 2 indicates that the user specifies on Record TFAT16A the fraction of each application that is intercepted on plant foliage, while FAM = 3 indicates that the model will calculate the interception of the application based on the canopy filtration parameter FILTRA on Record TFAT16B. If FAM=4, pesticide is applied to the soil surface in a granular formulation; release of pesticide from granules is then estimated using the rate constants input on Record TFAT16C.

Records TFAT17A through TFAT17D describe the penetration of pesticide applications into the canopy, and are required only if FAM = 2 or 3. Input of these records will depend upon the value of KANOPT on Record TFAT15. If KANOPT = 1, the user specifies how each application penetrates the canopy on Records TFAT17A and TFAT17B. If KANOPT = 2, the model will calculate canopy penetration based on data in Record TFAT17C. Record TFAT17D is required for KANOPT = 1 or 2, and describes the decay and washoff of pesticide on plant foliage.

The final two records in the application data group contain data needed to describe the volatilization of the pesticide from soil and water. Record TFAT18 consists of the degradation rate constant for the pesticide in ponds, the diffusion coefficient in water, and the initial concentration in ponds. Record TFAT19 contains the reference height for wind measurements, the pesticide diffusion coefficient in air, and the initial atmospheric concentration of pesticide vapor.

The soils data group (Records TFAT20 - TFAT26A) describes the properties of each soil horizon in the habitat. Record TFAT20 is a 1 to 80 character title for soils data. Record TFAT21 contains data for the entire soil column, including the number of soil layers modeled, the soil core depth, and various option flags for input of soil properties. Record TFAT22A is input only if the model is to calculate the partition coefficient for the pesticide in soil (KDFLAG = 1). Soil properties are then described for various horizons in the soil column; soil properties for all layers within a horizon are assumed to be uniform. Record TFAT23 is the number of horizons

NHORIZN, while Record TFAT24 describes the soil properties for each horizon and is repeated NHORIZN times. Records TFAT25A through TFAT25D are then input depending upon the bulk density option (BDFLAG) selected on Record TFAT21. Finally, Records TFAT26 and TFAT27A are used to assign initial pesticide levels, if applicable, to each soil layer.

Output options are selected on Records TFAT28, TFAT29, and TFAT30. Record TFAT28 is used to select the output frequency for hydrologic summaries, pesticide summaries, and concentration profiles; these may be printed daily, monthly, or annually for various numbers of soil layers. Records TFAT29 and TFAT30 specify which variables are to be written out as time series. Labels used to select variables for time series output are shown in Table 5.6.

5.2.5 Plant Growth and Translocation Location Modules

The data required for both the plant growth (PLTGRN) and plant translocation (PLTRNS) module, are defined in a single file. The order of parameter input is illustrated in Table 5.7. These parameters have to be provided for each crop within each habitat. The number of crops within each habitat is defined in the TFAT input file (see Table 5.5). The order that these crop parameters are read in is the same order as defined for the TFAT module (in order of the succession of the crops). Note that the planting dates and crop succession information have been retained in TFAT. Only information specific to plant growth simulation is read in by the PLTGRN module.

If more than one habitat is being simulated, all of the parameters for crops in the first habitat are defined, followed by all of the crops in the second habitat, etc. If the same crop appears in more than one habitat, it must be redefined in each habitat in which it appears.

Each record of this input file expects only one parameter to be defined. The first 24 spaces of each record are available for the user to insert notes as to what the parameter is--this field of 24 characters is ignored by the software. The only exception to this rule is that the first record (PL1) must have the label 'PLANT' in the first 5 columns to indicate that a new plant is being defined.

The initial condition values, records PL17 through PL27, are used if some non-zero initial conditions exist for plant biomass and for contaminant within the plant biomass; otherwise, these values can be set to zero (or, equivalently, contain a blank field).

5.2.6 Input Data for the Terrestrial Animal Exposure Module (APUM)

This section describes the format and content of the input file required for the Terrestrial Animal Exposure Module (APUM). APUM data records may be subdivided into four data groups:

- Soil Animal Data (Records APUM1 - APUM9)
- Higher Animal Data (Records APUM10-APUM21)
- Predation Data (Records APUM22-APUM26)
- Output Specifications (Records APUM27-APUM29)

The specific contents and formats for these data records are shown in Table 5.8. A general discussion of the types of data and user options for each data group is provided in the following paragraphs.

The soil animal data group (Records APUM1-APUM9) describes the uptake and movement of animals living in or on the soil in each habitat. These animals are exposed to chemicals by ingestion and by contact with soil, and their uptake of pesticide is modeled using bioconcentration factors. Soil dwelling animals may move between soil horizons, but cannot move between habitats. They also may not prey on other animals. The first Record (APUM1) in this group contains a descriptive run title used to identify input and output files. Records APUM2 and APUM3 contain the number of soil horizons and the number of soil animals respectively in each habitat. Note that number of soil horizons NSCOM must be less than or equal to the number of TFAT module soil horizons in the corresponding habitat. Records APUM4 through APUM9 contain specific uptake and movement data and are repeated for each soil animal in each habitat. Soil animals are identified for output and predation by the label ALABEL read on Record APUM4.

Movement of each soil animal may be modeled by one of three options, as specified by the variable ICOLD on record APUM7. If ICOLD = 0, the animal is modeled as a population distributed among soil horizons. The distribution of the population changes over time as determined by the horizon-movement transition matrix for the animal. This option requires input of the transition matrix on Record APUM8 and the initial population distribution on Record APUM9. If ICOLD < 0, the animal is modeled as a population with a steady-state distribution. The transition matrix on Record APUM8 is then not required, and the population distribution will remain constant as input on Record APUM9. Finally, if ICOLD > 0 the animal moves randomly from horizon to horizon as determined from its previous location and the transition matrix. ICOLD in this case is the initial horizon location of the animal. This option requires input of the transition matrix (Record APUM8) but does not require Record APUM9.

The higher animal data group (Records APUM10-APUM21) describes the uptake and movement of animals which prey on other animals and move between habitats. Modeling of these animals requires a specific breakdown of food preferences, assimilation factors, and interhabitat movement parameters. The first data Record APUM10 contains the number of higher animals modeled. The remaining records (APUM11-APUM21) contain specific uptake and movement data and are repeated for each higher animal. Record APUM11 is a unique 1 to 20 character label identifying the animal for output and predation.

As in the case of soil animals, one of three options for modeling movement between habitats may be specified using the parameter IHOLD on Record APUM19. If IHOLD = 0, the animal is modeled as a population distributed among habitats as determined from the habitat transition matrix. This option requires input of the habitat transition matrix on record APUM20 and the initial population distribution on record APUM21. If IHOLD < 0 , the distribution of the animal population is at steady state as specified on record APUM21. Under this option the habitat transition matrix on record APUM20 is not required. Finally, if IHOLD > 0 the animal moves randomly as determined from its previous location and the transition matrix. IHOLD in this case is the initial location of the animal. This option requires record APUM20 but does not require record APUM21.

The predation data group (Records APUM22-APUM26) describes the predator-prey relationships between various animals. Record APUM22 contains the number of predator-prey pairs to be described in Records APUM23-APUM26. Record APUM23 contains the label for the predator, and must correspond to a previously defined higher animal label input on Record APUM11. Record APUM24 is the name of the prey and must correspond to a label input on Records APUM4 or APUM11. Prey may consist of either soil animals or higher animals. The remaining records describe the preference factor, assimilation efficiency and capture probabilities for the predator-prey pair. Note that Records APUM23 through APUM26 must be repeated for each predator-prey pair; if an animal has 3 prey, 3 sets of Records APUM23-APUM26 are required.

The final data group (Records APUM27-APUM29) consists of various output options. Record APUM27 is a 4-character label selecting the frequency at which detailed dosage breakdowns are written; these may be written daily, monthly, or annually. The model also has the ability to write out time series of selected variables for plotting. The variables which are to be written out are specified by labels input on Record APUM29 (see Table 5.8 for the labels corresponding to model output variables).

5.2.7 Input Data for the Monte Carlo Module (MC)

The Monte Carlo module uses one batch input file to specify the distributions of variables and to select output options. This section describes the format of this input file and the available user options.

Note that when Monte Carlo simulations are performed, only one TEEAM habitat can be used in the system configuration.

The Monte Carlo input file consists of data records and two types of general utility records. The first type of utility record is the comment line, indicated by the presence of three asterisks ('***') as the first non-blank characters in the line. Comment lines may be inserted anywhere in the data set. The second type of utility record is the END line used by the code to mark the end of specific data groups. These records are indicated by the word 'END' in the first three columns of the input line, and should be used only where specified in the following discussion.

Monte Carlo input data are comprised of four data groups:

- Simulation control parameters (Records MC1-MC2)
- Input distribution parameters (Records MC3-MC4)
- Output options (Records MC5-MC6)
- Correlated variable input (Records MC7-MC8)

Data are read sequentially starting with Data Group 1 and ending with Data Group 4. Specific formats for each Data Group are shown in Tables 5.9 and are discussed below.

The simulation control data group consists of two records of data describing simulation options. Record MC1 contains the (alphanumeric) title for the run and is used to label the output. Record MC2 contains the number of Monte Carlo runs to be used in the simulation.

The input distribution group consists of one line of data (Record MC3) for each model parameter that is to be randomly varied. The first entry on Record MC3 is a label, of length up to 20 characters, used to identify these parameters. The labels which may be used are shown on Table 5.10. The second entry is the array index INDX for variables which are arrays used to indicate which array element is to be randomly varied. Variables dimensioned by HORIZON in Table 5.10 require the soil horizon number for INDX, variables dimensioned by CROP require the crop number, while variables dimensioned by ANIMAL require the animal number. Variables dimensioned by NAPP require the application number. Crops and animals are numbered in the order in which they are input in the TFAT and APUM data files. The remaining data on Record MC3 consist of frequency distribution parameters for the selected variables, as shown in Table 5.9. After a Record is provided for each desired random variable, an END card (Record MC4) must be supplied to mark the end of this data group. Note that by setting the distribution flag VAR(5) to 0 the user can specify a variable as a constant. In this case, the mean value of the variable (VAR(1)) will be used in all simulations. This option allows the user to randomly vary parameters without extensive modification of the input file.

The output options data group specifies the statistical output options for each variable to be written out. Note that the TEEAM Monte Carlo module calculates output statistics for variables which are time series' by taking the maximum value of the variable averaged over a specified period. Thus, if an averaging period of N-days is input, the model will select the maximum N-day average value from each Monte Carlo run for calculations of summary statistics and cumulative distributions. This moving average approach was used because lethal dosage feeding studies are often conducted over a known number of days. Thus, if the user wishes to create a distribution of the highest average daily dosage of chemical to the animal over a 10-day period, then 10 days would be selected as the averaging period.

If the maximum daily value of dosage or whole body concentration is desired, the user can specify one day as the averaging period. If the user desires the average of the entire time series, then the length of the time series would be chosen as the averaging period. The output data group consists of one line (Record MC5) for each output variable containing (1) a character label up to 20 characters long identifying the output variable, (2) an array index INDX indicating which array element is to be written out, (3) a flag indicating if a cumulative distribution should be plotted for this variable (selected by supplying "CDF" here), (4) a flag indicating if values of the variable are to be written out for each Monte Carlo run (selected by supplying the word "WRITE" here), and (5) the number of days used in calculating moving averages. The labels used to identify variables are shown on Table 5.8b. Variables dimensioned by HORIZON in Table 5.11 require the soil horizon number for INDX, variables dimensioned by CROP require the crop number, while variables dimensioned by ANIMAL require the animal number. Variables dimensioned by NAPP require the application number. A statistical summary table will be printed out for all variables selected in this data group. An END card (Record MC6) is supplied to mark the end of this Data Group after Record MC5 is input for each output variable.

The correlated variable data group is used to indicate which of the input variables specified in Data Group 2 are correlated. Note that only variables with normal and/or log normal distributions can be correlated. One line of data (Record MC7) is provided for each pair of correlated variables. The first two entries on this record are labels identifying the two variables that are correlated. These labels must correspond to Monte Carlo labels input on Record MC3. The third entry on these data lines is the value of the correlation coefficient. After a data line is supplied for each correlated pair of variables, an END card (Record MC8) must be provided to mark the end of the data group.

Table 5.1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP)

Variable	Description	Units
OPTION RECORDS EXESUP1 -- ANAME, STATS FORMAT (2A24)		
ANAME	Name of simulation option which can be one of the following list:	

Value	Module or variable
'TFAT'	Terrestrial fate and transport
'AERIAL SPRAY'	TFAT interface to FSCBG
'FSCBG'	Spray application
'PLTGRN'	Plant growth and translocation
'APUM'	Animal uptake and movement
'NHAB'	Number of habitats
'MONTE CARLO'	Monte Carlo module
'ENDRUN'	End of option's selection

Variable	Description	Units
STATS	Either "ON" or "OFF" for the modules or an integer value in columns 25-35 for the number of habitats. The following are the default values which are assumed if the module status is not explicitly defined.	

Module	Stats
TFAT	ON
AERIAL SPRAY	OFF
FSCBG	OFF
PLTGRN	ON
APUM	ON
MONTE CARLO	OFF
NHAB	1

Variable	Description	Units
FILE RECORDS EXESUP2 -- ANAME, FNAME FORMAT (2A24)		
ANAME	Label defining which input or output file is being defined. The following values of ANAME can be used and must be present if they are required.	

Table 5.1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP) (continued)

Variable	Description	Units
Value	When Required	File Represented
'PATH'	never required but is available as a convenience in defining file location	Path for following files.
'TFAT'	TFAT is ON	TFAT definition input file.
'PLTGRN'	PLTGRN is ON	Plant growth and translocation definition input file.
'METEOROLOGY'	always	Meteorological data (time series) input file.
'GRID DEFINITION'	AERIAL SPRAY is ON	Input file defining the spatial relationship between FSCBG output and TEEAM habitats.
'FSCBG OUTPUT'	AERIAL SPRAY is ON	Output of FSCBG simulation.
'APUMIN'	APUM is ON	Animal uptake and movement definition (input) file.
'MCIN'	MONTE CARLO is ON	Monte Carlo simulation definition (input) file.
'APUMOUT'	APUM is ON and MONTE CARLO is OFF	Animal model output file.
'ANIMAL TIME SERIES'	APUM is ON and MONTE CARLO is OFF	Animal time series output file.
'CONCENTRATIONS'	TFAT is ON and MONTE CARLO is OFF	TFAT contaminant concentrations output file.
'HYDROLOGY'	TFAT is ON and MONTE CARLO is OFF	TFAT hydrology output file.

Table 5.1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP) (continued)

Variable	Description	Units
Values	When Required	File Represented
'PESTICIDES'	TFAT is ON and MONTE CARLO is OFF	TFAT pesticides output file.
'TIME SERIES'	TFAT is ON and MONTE CARLO is OFF	TFAT, PLTGRN, and PLTRNS time series output file.
'ANIMAL TIME SERIES'	APUM is ON and MONTE CARLO is OFF	Animal model time series output file.
'MCOUT'	MONTE CARLO is ON	Monte Carlo output summary.
'MCOUT2'	MONTE CARLO is ON	Monte Carlo output of individual simulations.
'ENDFILES'	Always - at end of file definition to indicate that all necessary files have been defined.	--
FNAME	The name of the file defined by ANAME. If the path of a previous PATH is to be ignored the first character of FNAME must be '@'. If FNAME is a path (i.e. ANAME was defined as 'PATH') it should end with the character '\' (for MSDOS microcomputers).	--

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Global parameters record EXESUP3 -- ISDAY, ISMON, ISTYR, IEDAY, IEMON, IEYR
FORMAT (2X, 3I2, 10X, 3I2)

ISDAY	Starting day of month of simulation, e.g., 1 = 1st day of month.	--
ISMON	Starting month of simulation, e.g., 2 = February.	--
ISTYR	Starting year of simulation, e.g., 79.	--
IEDAY	Ending day of month of simulation, e.g., 31 = 31st day of month.	--

Table 5.1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP) (continued)

Variable	Description	Units
IEMON	Ending month of simulation, e.g., 12 = December.	--
IEYR	Ending year of simulation, e.g. 80.	--
Global parameters record EXESUP4 -- PFAC, SFAC, IPEIND, ANETD FORMAT (2F8.0, I8, F8.0)		
PFAC	Pan evaporation adjustment factor. This factor is multiplied by daily pan evaporation to estimate daily potential evapotranspiration (ET). If daily air temperatures are used to calculate ET, any dummy number can be input for PFAC (e.g., 0.75).	decimal
SFAC	Snow melt factor. Amount of melt per degree (°C) above freezing. Values of snow factor are in the order of 0.45. If snow melt is not to be calculated, enter 0.0 for SFAC.	cm/°C
IPEIND	Pan evaporation flag. If IPEIND = 0, pan evaporation data are read. If IPEIND = 1, temperature data are read and used to calculate potential ET. If IPEIND = 2, then pan evaporation, if available, is used in the meteorologic file; if not, temperature is used to compute potential ET.	--
ANETD	Minimum depth to which evaporation is extracted year round (e.g., 20) for all habitats.	cm
Global parameters record EXESUP5 -- DT FORMAT (6F8.0)		
DT(12)	Average length of daylight in each month. A total of 12 values (one for each month) are required and are input in two lines in the file.	hr/day
Trace Record EXESUP5 -- ANAME, STATS FORMAT (2A24)		
ANAME	The label 'TRACE'	--
STATS	The label 'OFF' if a subroutine trace is not desired or an integer value which is the depth of subroutine nesting to be displayed. If trace record EXESUP5 is not present, TRCLVL defaults to 3.	--

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE

Variable	Description	Units
Record FSCBG1--TITLE FORMAT (40A2)		
TITLE	A 1 to 80 character title for the FSCBG simulation	--
Record FSCBG2--ISW FORMAT (- list directed -)		
ISW (30)	Array of FSCBG option flags. Only options 1, 2, 5, 6, 18, 19, 21 and 22 are available. See Table 5.2b.	--
Record FSCBG3--IFWATR, WNGSPN, HGTCFT, DENLIQ FORMAT (- list directed -)		
IFWATR	Flag to identify if spray liquid base is water. If this flag is set equal to "1" or omitted, the program assumes the theoretical drop evaporation equations for water are to be used. If this parameter is set equal to "2", the program assumes the spray liquid is not water, but calculates a theoretical evaporation rate requiring these additional input parameters:	--
WNGSPN	Aircraft wingspan or helicopter rotor diam.	m
HGTCFT	Height of aircraft or ground sprayer above ground	m
DENLIQ	Density of drop liquid. If this parameter is omitted from the input data, the program defaults to a density of 1.0 gram per cubic centimeter.	g cm^{-3}
Record FSCBG4--AIRMOL, AIRPRS, FORMAT (- list directed -)		
AIRMOL	Molecular weight of air. If this parameter is omitted from the input data, the program uses 28.9644 as a default value.	g $mole^{-1}$

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
AIRPRS	Air pressure at the site altitude. If this parameter is omitted from the input data, the program uses 1013.25 millibars as a default value.	mb

***********************RECORD FSCBG4A1 IS REQUIRED*************************
if IFWATR = 1

Record FSCBG4A--RELHMO
FORMAT (- list directed -)

RELHMO	Average relative humidity above the canopy	percent

***********************RECORD FSCBG5A IS REQUIRED*************************
if ISW(1) is equal to 1

Record FSCBG5A--ARCRWT, ARCRSP
FORMAT (- list directed -)

ARCRWT	Aircraft weight	kg
ARCRSP	Aircraft or ground sprayer ground speed	ms^{-1}

***********************RECORD FSCBG5B IS REQUIRED*************************
if ISW(1) is equal to 0

Record FSCBG5B--WAKVEL
FORMAT (- list directed -)

WAKVEL	Wake settling velocity	ms^{-1}

***************RECORDS FSCBG6A1 AND FSCBG6A2 ARE REQUIRED******************
if ISW(2) is equal to 0

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
Record FSCBG6A1--DRPUPR FORMAT (- list directed -)		
DRPUPR(20)	Upper limits for drop-size categories, for up to 20 categories. These values must be input in descending order of diameter and the number of drop-size categories is determined by the program from the number of non-zero input values. If ISW(2) is equal to "0" or omitted, this array may be the mean diameter.	μm
Record FSCBG6A2--DRPLWR FORMAT (- list directed -)		
DRPLWR(20)	This parameter is an array specifying the lower limit of each drop-size category for the same number of drop-size categories input to the array DRPUPR. The lower limit of any drop size category cannot be zero ("0"). If the mean diameter is input to the array DRPUPR, this array is omitted from the input data.	μm
****************RECORDS FSCBG6B1 TO FSCBG6B5 ARE REQUIRED****************** if ISW(2) is equal to 1		
Record FSCBG6B1--DRPUPR FORMAT (- list directed -)		
DRPUPR(20)	Upper limits for drop-size categories, for up to 20 categories. These values must be input in descending order of diameter and the number of drop-size categories is determined by the program from the number of non-zero input values. If ISW(2) is equal to "0" or omitted, this array may be the mean diameter.	μm

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
Record FSCBG6B2--DRPLWR	FORMAT (- list directed -)	
DRPLWR(20)	This parameter is an array specifying the lower limit of each drop-size category for the same number of drop-size categories input to the array DRPUPR. The lower limit of any drop size category cannot be zero ("0"). If the mean diameter is input to the array DRPUPR, this array is omitted from the input data.	μm
Record FSCBG6B3--DRPPCT	FORMAT (- list directed -)	
DRPPCT(20)	Array containing the fraction of the total volume of material for each drop-size category subject to evaporation. Fracation from 0 to 1. The default value for each drop-size category is 1.	fraction
Record FSCBG6B4--AIRPRS, AIRMOL, VAPMOL, RELHMO	FORMAT (- list directed -)	
AIRPRS	Air pressure at the site altitude. If this parameter is omitted from the input data, the program uses 1013.25 millibars as a default value.	mb
AIRMOL	Molecular weight of air. If this parameter is omitted from the input data, the program uses 28.9644 as a default value.	g mole^{-1}
VAPMOL	Molecular weight of the vapor from the evaporating drops (Default = 18.015).	g mole^{-1}
RELHMO	Average relative humidity above the canopy.	percent

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
	************************RECORD FSCBG6B5 IS READ IF************************** IFWATR is equal to 2 (and ISW(2) = 1)	
Record FSCBG6B5--DFUSIV, HETLAT, THERMC, BCONST, CCONST FORMAT (- list directed -)		
DFUSIV	Diffusivity of evaporating vapor into air at the drop temperature. If this parameter is omitted from the input data and IFWATR equals "2," the program calculates DFUSIV, assuming the liquid is similar to water via the equation $\mathrm{DFUSIV} = .211 \cdot ((T_D+273.16)/273.16)^{1.94} \cdot (1013.25/\mathrm{AIRPRS})$ where T_D is the drop temperature approximated by the program.	$\mathrm{cm}^2\ \mathrm{sec}^{-1}$
HETLAT	Latent heat of vaporization at the drop temperature. If this parameter is omitted, the program calculates HETLAT, assuming the liquid is similar to water, via the equation $\mathrm{HETLAT} = 597.3 \cdot (273.16/(T_D+273.16))^{A} \cdot \mathrm{VAPMOL}$ where: $A = 0.107+3.67\times10^{-4} \cdot (T_D+273.16)$ T_D = drop temperature (°C) approximated by the program.	$\mathrm{cal\ mole}^{-1}$
THERMC	Thermal conductivity of the vapor into air at the drop temperature. If this parameter is omitted from the input data, the program calculates THERMC, assuming the liquid is similar to water, via the equation $\mathrm{THERMC} = A(1-(1.17-1.02(B/A)))\ \mathrm{VAPINF/AIRPRS}$ where: $A = 5.69\times10^{-5}+1.7\times10-7 \cdot \mathrm{DRPTMP}$ $B = 3.78\times10^{-5}+2.0\times10-7 \cdot \mathrm{DRPTMP}$ DRPTMP = calculated drop temperature (°K) VAPINF = calculated vapor pressure of vapor at infinity (mb) AIRPRS = barometric pressure (mb)	$\frac{\mathrm{cal}}{\mathrm{sec\ cm\ ^{\circ}K}}$

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
BCONST	Constant used in the equation that describes the vapor pressure of the non-water liquid as a function of temperature via the expression	decimal

vapor pressure (in Hg) = exp (BCONST-CCONST/T_D)

where T_D is the drop temperature (°C) approximated by the program. The default value for BCONST is 21.07.

Variable	Description	Units
CCONST	Factor used in the equation that describes the vapor pressure of the non-water liquid as a function of temperature (Default = 5249.9)	°K

***********************RECORD FSCBG6C1 IS REQUIRED************************
if ISW(2) is equal to 2

Record FSCBG6C1--DRPPCT
FORMAT (- list directed -)

Variable	Description	Units
DRPPCT(20)	Array containing the fraction of the total volume of material for each drop-size category subject to evaporation. Fraction from 0 to 1. The default value for each drop-size category is 1.	fraction

******************RECORDS FCBG6C2 TO FCBG6C4 ARE REQUIRED*****************
if ISW(2) is equal to 2

DAU, DBU, and DCU

Arrays of coefficients of the quadratic equation that gives the drop diameter in micrometers as a function of time above the canopy. There are a maximum of 20 values for each array. The order of values in each array is in descending order of drop size. There are no default values for these parameters.

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
	The number of drop size categories is determined by the number of non-zero values of DAU and DBU input. These equations are applicable from release time (T=0) up until the fraction of material given by DRPPCT has been evaporated. When the fraction of material given by DRPPCT has been evaporated, the program will switch to the coefficients EAU, EBU, and ECU. Also, if the quadratic given by DAU, DBU, and DCU is not valid beyond a certain time (drop size begins to grow with increasing time), the program will switch to EAU, EBU, and ECU. The DAU, DBU, DCU equation is -	

$$\mathrm{DROP} = \mathrm{DAU(J)} + \mathrm{DBU(J)} \cdot \mathrm{T} + \mathrm{DCU(J)} \cdot \mathrm{T}^2$$

where:

DROP is diameter in micrometers

J is the index over drop size categories

T = 0 through T1, where T1 is the time at which -

$$\mathrm{DAU(J)+DBU(J)} \cdot \mathrm{T1+DCU(J)} \cdot \mathrm{T1}^2 = (\mathrm{DAU(J)}^3 \cdot (1-\mathrm{DRPPCT(J)}))^{.3333}$$

or

$$\mathrm{DAU(J)+DBU(J)} \cdot \mathrm{(T1+DT)+DCU(J)} \cdot \mathrm{(T1+DT)}^2 > \mathrm{DAU(J)+DBU(J)} \cdot \mathrm{T1+DCU(J)} \cdot \mathrm{T1}^2$$

Record FSCBG6C2--DAU

FORMAT (- list directed -)

Variable	Description	Units
DAU(20)	First coefficient in equation to compute drop diameter in each drop-size category above the canopy as a function of time.	******

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
Record FSCBG6C3--DBU	FORMAT (- list directed -)	
DBU(20)	Second coefficient in equation to compute drop diameter in each drop-size category above the canopy as a function of time.	μm/sec
Record FSCBG6C4--DCU	FORMAT (- list directed -)	
DCU(20)	Third coefficient in equation to compute drop diameter in each drop-size category above the canopy as a function of time.	$\mu m/sec^2$

***************RECORDS FSCBG6C5 TO FSCBG6C7 ARE REQUIRED*******************
if ISW(2) is equal to 2

EAU, EBU, AND ECU

Arrays of coefficients of the quadratic equation that gives the drop diameter in micrometers as a function of time above the the canopy after the fraction material given by DRPPCT has been evaporated down to a minimum of 5 micrometers. There are a maximum of 20 values for each array. The order of values in each array is in descending order of drop size. If not input, the program keeps the drop size constant after time T1 (DRPPCT material evaporated) given under DAU, DBU, DCU. The EAU, EBU, ECU equation is -

```
DROP = EAU(J) + EBU(J)*T + ECU(J*T**2
```

where:

DROP is the diameter in micrometers.

J is the index over drop size categories.

T is the time in seconds from release time and is > = time T1.

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
Record FSCBG6C5--EAU	FORMAT (- list directed -)	
EAU(20)	Alternate first coefficient in equation to compute drop diameter in each drop-size category above the canopy as a function of time. Used when liquid within drop-size category had vaporized to minimize size.	μm
Record FSCBG6C6--EBU	FORMAT (- list directed -)	
EBU(20)	Alternate second coefficient in equation to compute drop diameter in each drop-size category above the canopy as a function of time. Used when liquid within drop-size category had vaporized to minimize size.	μm sec^{-1}
Record FSCBG6C7--ECU	FORMAT (- list directed -)	
EAU(20)	Alternate third coefficient in equation to compute drop diameter in each drop-size category above the canopy as a function of time. Used when liquid within drop-size category had vaporized to minimize size.	μm sec^{-2}
********************THE REMAINING RECORDS ARE READ***********************		
Record FSCBG7--NSOURC	FORMAT (- list directed -)	
NSOURC	Total number of line sources (spray lines). The program is capable of processing a maximum of 60 line sources. If this value is input as "0" or omitted from the input data, the program defaults to a value of "1".	--

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
Record FSCBG8--Q FORMAT (- list directed -)		
Q(30)	This parameter specifies the spray emission rate for the line sources in units of grams per meter, or gallons per acre, depending on the input parameter SWATH. If the parameter SWATH is greater than zero, the program assumes Q is in gallons per acre and the area sprayed is sprayed in lines of an equal distance (SWATH) apart. If the spray lines are not uniform or the area is not regular, input Q in units of grams per meter and set the parameter SWATH equal to "0" or omit SWATH from the input data. If the parameter Q is input as "0" or omitted from the input data, the program defaults to a value of "1". If any Q(2) through Q(NSOURC) are omitted or zero, the program will default the respective Q to the value of the previous Q in the array.	$g\ m^{-1}$ or gallon $acre^{-1}$
Record FSCBG9--SWATH, DELTAH FORMAT (- list directed -)		
SWATH	Distance between spray lines when Q is input in units of gallons/acre. If Q is input in grams/meter omit SWATH or set SWATH to 0.0 (Default = 0.0).	m
DELTAH	Depth of each volume source for calculation of concentration and/or dosage from gas evaporated. If there is no evaporation, this parameter is not used. (Default = 1.0). If >0.0, the program assumes this is the decrement in height to use for gas calculations from the release height to the ground (or the drop stops evaporating or completely evaporates). If < 0.0, the program assumes the absolute value is the number of gas sources you desire from the release height to the ground and divides this height into the number of source intervals specified.	m

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
Record FSCBG10--TAU, TAU0 FORMAT (- list directed -)		
TAU	Time to spray cloud stabilization. If this parameter is input as "0" or omitted from the input data, the program defaults TAU to 2.5 seconds.	sec
Record FSCBG11--SIGXYZ, DECAY, XLRZ, DELU FORMAT (- list directed -)		
SIGXYZ	Initial standard deviation of source material distribution along the spray line. If this parameter is input as "0" or omitted from the input data, the program defaults SIGXYZ to WNGSPN/4.3.	m
DECAY	Coefficient of time dependent exponential decay for the removal of material due to chemical or physical processes.	sec
XLRZ	Lateral and vertical reference distance. This parameter is normally calculated by the program. However, if XLRZ is input greater than or equal to zero, the input value is used.	m
DELU	Wind-speed sheer above the canopy (Default = 0).	$m\ sec^{-1}$
Record FSCBG12--HM, THETA, DAREA, BETA1 FORMAT (- list directed -)		
HM	Mixing layer height above ground.	m
THETA	This parameter specifies the wind direction (direction from which wind is blowing) in degrees, measured clockwise from 0 degrees (north).	deg
BETA1	Ratios of Langrangian to Eularian time-scales used in the correction factor on the standard deviations of the horizontal and vertical wind directions. Suggested value, if used, is 1.0 (default is 0.0).	decimal

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (continued)

Variable	Description	Units
Record FSCBG13--DX	FORMAT (- list directed -)	
DX(60)	Source X (East-West) Coordinates -- This parameter is an array specifying the start and end X coordinate of each line source. Input the start followed by the end X coordinate for each source. Either end of the line may be the start coordinate. X must increase from west to east.	m
Record FSCBG14--DY	FORMAT (- list directed -)	
DY(60)	Source Y (North-South) Coordinates -- This parameter is an array specifying the start and end Y coordinate of each line source. Input the start followed by the end Y coordinate for each source. Y must increase from south to north.	m
Record FSCBG15--PCTMAT	FORMAT (- list directed -)	
PCTMAT(20)	Input these values in descending order of drop-size categories.	fraction
Record FSCBG16--VSGAM	FORMAT (- list directed -)	
VSGAM(2)	Array of two settling velocities that specify the settling velocities that break the curve of surface reflection coefficients given by GAMA, GAMB, and GAMC into three parts. Settling velocities (VS) greater than or equal to VSGAM(1) use GAMA(1), GAMB(1), and GAMC(1) to calculate the surface reflection coefficient. VS values less than VSGAM(2) use GAMA(2), GAMB(2), and GAMC(2) to calculate the surface reflection coefficient. VS values less than VSGAM(2) use GAMA(3), GAMB(3), and GAMC(3). Default values for VSGAM are provided only if VSGAM is omitted from the input list. Default values are VSGMC(1) = 0.04 and VSGAM(2) = 0.012.	m $\sec^{-1}$

Table 5.2a. INPUT FORMATS FOR FSCBG MODULE (concluded)

Variable	Description	Units

Record FSCBG17--GAMA, GAMB, GAMC
FORMAT (- list directed -)

GAMA, GAMB, GAMC - Arrays of coefficients of the quadratic equation that gives the fraction of material reflected at the surface as a function of the drop settling velocity.

$$\text{Fraction} = GAMA(J) + GAMB(J) + GAMC(J) \cdot VS^{2}$$

where: VS is the drop settling velocity in meters/sec

$$J = \begin{cases} 1, & \text{if } VS \geq VSGAM(1) \\ 2, & \text{if } VS \geq VSGAM(2) \text{ and } VS < VSGAM(1) \\ 3, & \text{if } VS < VSGAM(2) \end{cases}$$

Three coefficients of GAMA, GAMB, and GAMC each must be input. The first value of each array is for settling velocities greater than or equal to VSGAM(1). The second value of each array is for settling velocities less than VSGAM(1) and greater than or equal to VSGAM(2). The third value of each array is for settling velocities less than VSGAM(2). The default values for the three arrays are:

GAMA(1) = 0.75, GAMA(2) = 0.83465302, GAMA(3) = .91639996
GAMB(1) = -2.5, GAMB(2) = -6.9031391, GAMB(3) = -22.357124
GAMC(1) = 0.00, GAMC(2) = 57.4092560, GAMC(3) = 821.426510

Variable	Description	Units
GAMA(3)	First coefficient to calculate fraction of material reflected at the surface as a function of drop settling velocity.	fraction
GAMB(3)	Second coefficient to calculate fraction of material reflected at the surface as a function of drop settling velocity.	fraction sec m^{-1}
GAMC(3)	Third coefficient to calculate fraction of material reflected at the surface as a function of drop settling velocity.	fraction sec^{2} m^{-2}

Table 5.2b. EXPLANATION OF FSCBG OPTIONS (ISW VALUES)

ISW(1) - Wake settling velocity option.

If = 0, the program assumes the wake settling velocity WAKVEL is being input

If = 1, the program assumes the wake settling velocity is to be calculated from the input parameters - ARCRWT, AIRDEN, WNGSPN and ARCRSP.

ISW(2) - Evaporation model option

If = 0, The evaporation model is not executed. The program assumes there is no change in drop size with time.

If = 1, The evaporation model is executed. The program calculates the rate of change of drop size with time.

If = 2, The evaporation model is not executed. The program assumes the user inputs the equations of the rate of change of drop size with time.

ISW(5) - Print evaporation model (ISW(2)) calculations option.

If = 0, Evaporation model calculations are not printed. This includes all calculations under ISW(2).

If = 1, The evaporation model calculations are printed in the form of quadratic equations only.

If = 2, The same as 1 and calculations at approx. one meter height intervals are printed.

If = 3, The same as 1, but calculations at all height intervals are printed.

If = 4, The same as 3, but additional tables giving the accuracy of the regression are printed.

If = 5, The same as 4, but debug calculations are also printed. Only use a few drop size categories due to the large volume of print output.

ISW(6) - Dosage Model Option.

If = 0, The Dosage is not calculated.

If = 1, The Dosage is calculated and printed.

Table 5.2b. EXPLANATION OF FSCBG OPTIONS (ISW VALUES) (continued)

ISW(18)- Option to print dosage and or deposition by drop size category.

If = 0, Only the total over drop size categories is printed.

If = 1, Dosage and/or deposition for each drop size category is printed.

If = 2, Dosage and/or deposition for each drop size category as well as the sum over drop size categories is printed.

ISW(19)- Option to print dosage and/or deposition by gas versus drop or by volatile versus non-volatile material

If = 0, Only total dosage and/or deposition is printed.

If = 1, The program prints the contribution to the total dosage from evaporated (gaseous) material and from non-evaporated (drop) material separately. Deposition is non-evaporated material only.

If = 2, The program prints the contribution to the total dosage from evaporated (gaseous) material and from non-evaporated (drop) material separately and summed. Deposition is non-evaporated material only.

If = -1, The program prints the contribution to the total dosage and/or deposition from volatile and from non-volatile material separately. The fraction of volatile material is determined from the array DRPPCT, which gives the fraction of material in each drop size category subject to evaporation.

If = -2, The program prints the contribution to the total dosage, and/or deposition from volatile and from non-volatile material separately and summed.

Table 5.2b. EXPLANATION OF FSCBG OPTIONS (ISW VALUES) (concluded)

ISW(21)- Option to calculate drop dosage and/or deposition from evaporating drops using the new or old model. The old model assumed VS was constant with distance and used VS*X/U in the vertical term. The new model uses (A+B*X+C*X**2)*X/U in the vertical term. This option is not applicable when ISW(2) = 0.

If = 0, The new model is executed. Results for dosage and deposition are returned as zero if the program calculated maximum distance for deposition is exceeded or for deposition, if negative deposition occurs.

If = 1, The new model is executed, but the maximum distance provision is relaxed.

If = 2, The old model is executed. VS rather than A+B*X+C*X**2 is used in the vertical term. There are no maximum distance restrictions.

ISW(22)- Option to produce deposition output in units of mass and length depending on ISW(9) and ISW(11), in number of drops per square meter and in drop volume mean diameter. This option is used only for ISW(18) > 0. ISW(9) must not be entered as zero if ISW(22) is set > zero.

Remaining options are set to the following values in TEEAM:

ISW	Value
3	0
4	1
7	0
8	1
9	1
10	0
11	0
12	0
13	1
14	1
15	0
16	0
17	0
20	0

Explanation of these options is given in the FSRED2 subroutine of the TEEAM code.

Table 5.3. INPUT FORMATS FOR THE SPRAY GRID DEFINITION MODULE

Variable	Description	Units
**************************RECORD GRID1 REPEATS**************************** FOR ALL HABITATS		
RECORD GRID1--XSW, YSW, XNE, YNE FORMAT (4F8.0)		
XSW	Southwest coordinate of habitat.	m
YSW	Southwest coordinate of habitat.	m
XNE	Northeast coordinate of habitat.	m
YNE	Northeast coordinate of habitat.	m
	(Note: X must increase from west to east, Y must increase from south to north)	
RECORD GRID2--MXPNTS, MYPNTS FORMAT (2I8)		
MXPNTS	Number of grid points in E-W transect.	--
MYPNTS	Number of grid points in N-S transect.	--
RECORD GRID3--X(1), GDX FORMAT (2F8.0)		
X(1)	Initial x-coordinate of FSCBG receptor grid	m
GDX	Increment between FSCBG receptor grid x-coordinates	m
RECORD GRID4--Y(1), GDY FORMAT (2F8.0)		
Y(1)	Initial y-coordinate of FSCBG receptor grid	m
GDY	Increment between FSCBG receptor grid y-coordinates	m
RECORD GRID5--NDOSE FORMAT (I8)		
NDOSE	Number of aerial spray applications	--

Table 5.3. INPUT FORMATS FOR THE SPRAY GRID DEFINITION MODULE (continued)

Variable	Description	Units

***************************RECORD GRID6 REPEATS*****************************
FOR EACH APPLICATION

RECORD GRID6--SAPD, SAPM, IYRPLY
FORMAT (2X, 3I2)

SAPD	Spray application day	--
SAPM	Spray application month	--
IYRPLY	Spray application year	--

*************************RECORDS GRID7 TO GRID10****************************
REPEAT FOR EACH HABITAT

RECORD GRID7--SAM, SANOPT
FORMAT (2I8)

SAM	Pesticide application model flag. There are two options: SAM = 2 indicates the user supplies the fraction of the application that goes to the canopy, and SAM = 3 indicates the model calculates the canopy application.	--
SANOPT	Canopy penetration flag. SANOPT = 1 indicates user-supplied canopy penetration, and SANOPT = 2 indicates canopy penetration will be computed.	--

***********************RECORD GRID8A ONLY REQUIRED************************
IF SAM = 2, REPEAT FOR
EACH APPLICATION (NDOSE)

RECORD GRID8A--SERCAN(I)
FORMAT (F8.0)

SERCAN(I)	The fraction of application I which is applicable to the crop canopy	fraction

***********************RECORD GRID8B ONLY REQUIRED************************
IF SAM = 3

RECORD GRID8B--SILTRA
FORMAT (F8.0)

SILTRA	Filtration parameter for canopy application model	--

Table 5.3. INPUT FORMATS FOR THE SPRAY GRID DEFINITION MODULE (continued)

Variable	Description	Units
********************RECORDS GRID9A1 AND GRID9A2 ONLY********************* REQUIRED IF SANOPT = 1, REPEAT FOR EACH APPLICATION (NDOSE)		
RECORD GRID9A1--SDEPLV(I), SIS(I) FORMAT (I8, F8.0)		
SDEPLV(I)	Number of deposition levels in canopy for application I	--
SIS(I)	Thickness of each deposition level	cm
************************RECORD GRID9A2 REPEATS FOR************************* EACH DEPOSITION LEVEL J = 1, SDEPLV(I)		
RECORD GRID9A2--SRACDL FORMAT (F8.0)		
SRACDL (J,I)	Fraction of deposition occurring on canopy level J for application I	fraction
***********************RECORD GRID9B ONLY REQUIRED************************ IF SANOPT = 2		
RECORD GRID9B--SDIS, SETA FORMAT (2F8.0)		
SDIS	Thickness of canopy deposition layers	cm
SETA	Penetration model attenuation constant	cm^{-1}
RECORD GRID10--SLDKRT, SEXTRC FORMAT (2F8.0)		
SLDKRT	Decay rate constant for pesticide on plant foliage	$days^{-1}$
SEXTRC	Foliar extraction coefficient for pesticide washoff per cm of precipitation	--

Table 5.4. INPUT FORMATS FOR THE TFAT METEOROLOGY FILE

Variable	Description	Units
Record MET1--MM, MD, MY, PRECIP, PEVP, TEMP, SOLAR, WIND FORMAT (1X, 3I2, 5F10.0)		
MM	Month (i.e., 1 for January)	--
MD	Day of Month (i.e., 1)	--
MY	Year (i.e., 84)	--
PRECIP	Daily precipitation amount	cm
PEVP	Daily potential evaporation. If a value of -99 is entered, the model will estimate PEVP from the air temperature and daily hours of sunshine for the month.	cm
TEMP	Air temperature	degrees C
SOLAR	Solar radiation	langleys
WIND	Mean wind speed at the reference height ZWIND (on Record TFAT19)	cm s^{-1}

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT)

Variable	Description	Units
********************ALL TFAT RECORDS ARE REPEATED AS********************** A SET FOR EACH HABITAT		
Record TFAT1--TITLE FORMAT (A80)		
TITLE	A 1 to 80 character title for the TFAT simulation.	--
Record TFAT2--HTITLE FORMAT (A80)		
HTITLE	This card provides a comment line of 80 characters for the user to input information regarding hydrology parameters.	--
Record TFAT3--INICRP, ISCOND, NPTIME, AFIELD FORMAT (3I8, F8.0)		
INICRP	User specified initial crop number if simulation date is before first crop emergence date (see record TFAT10).	--
ISCOND	User specified surface condition after harvest corresponding to INICRP (either fallow cropping, or residue, corresponding to dimensionless integer of 1, 2 or 3).	--
NPTIME	Number of time steps per day used in pond water balance and chemistry calculations (must be $\geq$ 1).	days
AFIELD	Area of the habitat (plan view).	ha
Record TFAT4--KSAT, HFPOND, PDEPTH, TC, ARAIN, BRAIN FORMAT (6F8.0)		
KSAT	Saturated hydraulic conductivity of surface soils.	cm hr^{-1}
HFPOND	Green-Ampt suction parameter.	cm
PDEPTH	Initial pond depth.	cm

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
TC	Average runoff time of concenration for the habitat.	hours
ARAIN	Coefficient A in rainfall-duration curve: duration = A(precip)^{B}	hr cm^{-B}
BRAIN	Coefficient B in the rainfall-duration curve	--
Record TFAT5--ASOIL, BSOIL FORMAT (2F8.0)		
ASOIL	Constant in relationship between air temperature and soil surface temperature: TSOIL = ASOIL + (BSOIL)(TAIR)	degrees C --
BSOIL	Slope in the relationship between air temperature and soil surface temperature.	--
Record TFAT6--ERFLAG FORMAT (I8)		
ERFLAG	Erosion flag. If erosion losses are not to be calculated, ERFLAG = 0, otherwise ERFLAG = 1.	--
Record TFAT7--USLEK, USLELS, USLEP, AFIELD, (Only if ERFLAG = 1; DO NOT include this card if ERFLAG = 0). FORMAT (4F8.0)		
USLEK	Universal soil loss equation (K) soil erodibility parameter (e.g., 0.15).	--
USLELS	Universal soil loss equation (LS) topographic factor (e.g., 0.14).	--
USLEP	Universal soil loss equation (P) supporting practice factor (e.g., 1.0).	--
AFIELD	Area of field or plot.	ha
Record TFAT8--NDC FORMAT (I8)		

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
NDC	Number of different crops used in the simulation (minimum of 1).	--
Record TFAT9--ICNCN, CINTCP, AMXDR, COVMAX, ICNAH, CN, USLEC, WFMAX FORMAT (I8, 3F8.0,I8, 3(1X, I3), 3(1X, F3.0), F8.0) NOTE: One record each must be read in to match the total number of crops (NDC).		
ICNCN	Crop number.	
CINTCP	Maximum interception storage of the crop.	cm
AMXDR	Maximum active root depth of the crop.	cm
COVMAX	Maximum areal coverage of the crop at full canopy.	percent
ICNAH	Soil surface condition after crop harvest (1 = fallow, 2 = cropping, 3 = residue).	--
CN	Runoff curve number for the antecedent soil water condition II, for fallow, crop, and residue fractions of the growing season (e.g. 86, 78, 82).	--
USLEC	Universal soil loss equation cover management factor. Three values must be entered in the same order as (CN), fallow, crop, and residue. Values only are required if ERFLAG = 1. Leaving them in the input stream will have no effect if ERFLAG = 0 (e.g., 0.20)	--
WFMAX	Maximum dry foliage weight of the crop at full canopy . Only required if the exponential filtration model is used for pesticide application (values of WFMAX will not affect the simulation if FAM = 1, 2, or 4. See record TFAT15.	$kg\ m^{-2}$
Record TFAT10--NCPDS FORMAT (I8)		
NCPDS	Number of cropping periods in the simulation (minimum of 1). If three cropping years of	--

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
	continuous corn are simulated, NCPDS = 3. If two winter cover crops are in the middle of the three years of corn, NCPDS = 5.	
Record TFAT11--EMD, EMM IYREM, MAD, MAM, IYRMAT, HAD, HAM, IYRHAR, INCROP FORMAT (2X, 3I2, 2X, 3I2, 2X, 3I2, I8) NOTE: One card each must be read in to match the total number of cropping periods (NCPDS).		
EMD	Day of month of crop emergence (e.g., 20).	--
EMM	Month of crop emergence (e.g., 4).	--
IYREM	Year of crop emergence (e.g., 82).	--
MAD	Day of month of crop maturation (e.g., 15).	--
MAM	Month of crop maturation (e.g., 10).	--
IYRMAT	Year of crop maturation (e.g., 82).	--
HAD	Day of month of crop harvest (e.g., 20).	--
HAM	Month of crop harvest (e.g., 10).	--
IYRHAR	Year of crop harvest (e.g., 82).	--
INCROP	Crop number of crop growing in current period (e.g., 1).	--
**********************END OF HYDROLOGY AND CROP DATA**********************		
Record TFAT12--PTITLE FORMAT (A80)		
PTITLE	This card provides a comment line of 80 characters for the user to input information regarding pesticide parameters.	--
Record TFAT13--NAPS FORMAT (I8)		
NAPS	Number of pesticide applications (minimum of 1). If no applications are desired in TFAT set TAPP (next record)	--

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
	to zero for this one required application, or set the date of application beyond the end of the simulation _________ date.	
Record TFAT14--APD, APM, IAPYR, TAPP, DEPI, CGRAN FORMAT (2X, 3I2, 3F8.0) NOTE: One card should be entered for each application up to the number of applications (NAPS).		
APD	Day of the month of pesticide application (e.g., 10).	--
APM	Month of pesticide application (e.g., 5).	--
IAPYR	Year of pesticide application (e.g., 82).	--
TAPP	Total pesticide or granule application.	kg/ha
DEPI	Depth of pesticide incorporation.	cm
CGRAN	Concentration of pesticide in granules (required only for granule applications, FAM = 4).	g/g
Record TFAT15--FAM, KANOPT FORMAT (2I8)		
FAM	Pesticide application model. There are four options: FAM = 1 indicates application to soil only, FAM = 2 indicates the user supplies the fraction of the application that goes to the canopy, FAM = 3 indicates the model calculates the canopy application, and FAM = 4 indicates application of granules to the soil surface.	--
KANOPT	Canopy penetration option, KANOPT = 1 indicates user-supplied canopy penetration, and KANOPT = 2 indicates the model will compute canopy penetration.	--
Record TFAT16A--PERCAN (I) FORMAT (F8.0)		
	Required only if FAM = 2; repeat for each application (NAPS times).	

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
PERCAN (I)	The fraction of application I which stays on the crop canopy.	fraction
Record TFAT16B--FILTRA FORMAT (F8.0)		
	Required only if FAM = 3 (model computes canopy application).	
FILTRA	Filtration parameter for canopy application model.	m^2 kg^{-1}
Record TFAT16C--GKWET, GKDRY FORMAT (2F8.0)		
	Required only if FAM = 4 (granule application).	
GKWET	Granule pesticide decay constant when granule is immersed in water.	$days^{-1}$
GKDRY	Granule pesticide decay constant when granule is dry.	$days^{-1}$
*********************RECORDS TFAT17A AND TFAT17B ARE********************* REPEATED FOR EACH APPLICATION		
Record TFAT17A--NDEPLV(I), DIS(I) FORMAT (I8, F8.0)		
	Required only if FAM = 2 or 3 and KANOPT = 1.	
NDEPLV(I)	Number of deposition levels in canopy for application I.	--
DIS(I)	Thickness of each deposition level.	cm
Record TFAT17B--FRACDL(J,I) FORMAT (F8.0)		
	Required only if FAM = 2 or 3 and KANOPT = 1; repeat for each deposition level J for application I.	
FRACDL (J,I)	Fraction of deposition occurring on canopy level J for application I.	fraction

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
**		
Record TFAT17C--BDIS, BETA FORMAT (2F8.0)		
	Required only if FAM = 2 or 3 and KANOPT = 2.	
BDIS	Thickness of canopy deposition layers.	cm
BETA	Penetration model attenuation constant.	cm^{-1}
Record TFAT17D--PLDKRT, FEXTRC FORMAT (2F8.0) Required only if FAM = 2 or 3.		
PLDKRT	Decay rate constant for pesticide on plant foliage.	$days^{-1}$
FEXTRC	Foliar extraction coefficient for pesticide washoff per cm of precipitation.	--
Record TFAT18--KDPOND,DWAT,CPND FORMAT (3F8.0)		
KDPOND	Degradation rate for pesticide in ponded water.	$days^{-1}$
DWAT	Diffusion coefficient of pesticide in water.	$cm^2\ day^{-1}$
CPND	Initial concentration of pesticide on ponded water (should = 0.0 if there is no initial ponding).	$g\ cm^{-3}$
Record TFAT19--ZWIND, DAIR, IH, CCAN FORMAT (4F8.0)		
ZWIND	Reference height for wind speed measurements in the MET data file.	m
DAIR	Diffusion coefficient of pesticide in air.	$cm^2\ day^{-1}$

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
KH	Dimensionless Henry's Law constant for pesticide (i.e., dissolved-vapor phase partition coefficient).	--
CCAN	Initial concentration of pesticide in the canopy atmosphere.	$g\ cm^{-3}$

*********************END OF PESTICIDE APPLICATION DATA*********************

Record TFAT20--STITLE
FORMAT (A80)

STITLE	This card provides a comment line of 80 characters for the user to input information regarding soils properties.	

Record TFAT21--CORED, UPTKF, NCOM2, BDFLAG, THFLAG, KDFLAG, HSWZT
FORMAT (2F8.0, 5I8)

CORED	Total depth of soil core	cm
UPTKF	Plant uptake efficiency factor; UPTKF = 0 indicates no plant uptake simulated, UPTKF = 1 indicates uptake is simulated and is equal to the crop transpiration rate, 0<UPTKF<1 (e.g., 0.10) indicates uptake is simulated and is a fraction of the crop transpiration rate. The value of this parameter will be ignored if the plant growth module (PLTGRN) is used.	--
NCOM2	Total number of simulation compartments in the soil core.	--
BDFLAG	Bulk density flag; BDFLAG = 0 indicates apparent bulk density known and entered, BDFLAG = 1 indicates apparent bulk density to be calculated and mineral bulk density entered.	--
THFLAG	Calculation flag for soil field capacity and wilting point water contents; THFLAG = 0 indicates water contents known and entered, THFLAG = 1 indicates water contents are not known and will be calculated.	--

Table 5.5. **INPUT FORMATS** FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
KDFLAG	Calculation flag for soil/pesticide sorption partition coefficients; KDFLAG = 0 indicates partition coefficients known and entered, BDFLAG = 1 indicates partition coefficients not known and will be calculated.	--
HSWZT	Switch for soil hydraulics; HSWZT = 0 indicates free draining soils, HSWZT = 1 indicates restricted draining soils.	--

Record TFAT22A--PCMC, SOL (Only if KDFLAG = 1, DO NOT include if KDFLAG = 0)
FORMAT (I8, F8.0)

Variable	Description	Units
PCMC	Calculation flag for model to estimate pesticide soil partition coefficients. There are three options: PCMC = 1, PCMC = 2, and PCMC = 3.	--
SOL	Pesticide solubility. The units vary according to the model (PCMC) selected; PCMC = 1, mole fraction; PCMC = 2, mg liter^{-1}; PCMC = 3, micromoles liter^{-1}.	--

Record TFAT23--NHORIZ
FORMAT (I8)

Variable	Description	Units
NHORIZ	Total number of soil horizons (minimum of 1).	--

*************REPEAT RECORDS TFAT 24-TFAT25D FOR EACH SOIL HORIZON***********

Record TFAT24--HORIZN, THKNS, BD, DISP, DKRATE, THETO, AD
FORMAT (I8, 6F8.0)

Variable	Description	Units
HORIZN	Soil horizon number.	--
THKNS	Soil horizon thickness	cm
BD	Soil bulk density (if BDFLAG = 0) and/or mineral bulk density (if BDFLAG = 1) in each horizon.	g cm^{-3}
DISP	Dispersion/diffusion coefficient for each soil horizon.	cm^2 day^{-1}

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
DKRATE	Pesticide decay rate in the soil horizon	days^{-1}
THETO	Initial soil water content in the horizon	$\text{cm}^3\ \text{cm}^{-3}$
AD	Soil horizon drainage parameter, used only if HSWZT = 1, otherwise, the value is ignored.	day^{-1}

Record TFAT25A--THEFC, THEWP, KD, OC (Only if THFLAG = 0 and KDFLAG = 0)
FORMAT (8X, 4F8.0)

Variable	Description	Units
THEFC	Field capacity soil water content of horizon	$\text{cm}^3\ \text{cm}^{-3}$
THEWP	Wilting point soil water content of horizon	$\text{cm}^3\ \text{cm}^{-3}$
KD	Sorption partition coefficient for soil horizon/pesticide combination	$\text{cm}^3\ \text{g}^{-1}$
OC	Organic carbon content of soil horizon. This value is also required if BDFLAG = 1.	percent

Record TFAT25B--THEFC, THEWP, OC (Only if THFLAG = 0 and KDFLAG = 1)
FORMAT (8X, 3F8.0)

Variable	Description	Units
THEFC	Field capacity soil water content of horizon.	$\text{cm}^3\ \text{cm}^{-3}$
THEWP	Wilting point soil water content of horizon.	$\text{cm}^3\ \text{cm}^{-3}$
OC	Organic carbon content of soil horizon. This value is also required if BDFLAG = 1.	percent

Record TFAT25C--SAND, CLAY, OC, KD (Only if THFLAG = 1 and KDFLAG = 0)
FORMAT (8X, 4F8.0)

Variable	Description	Units
SAND	Percent sand in soil horizon.	percent
CLAY	Percent clay in soil horizon.	percent
OC	Organic carbon content of soil horizon. This value is also required if BDFLAG = 1.	percent

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
KD	Sorption partition coefficient for soil horizon/pesticide combination.	$cm^3\ g^{-1}$
Record TFAT25D--SAND, CLAY, OC (Only if THFLAG = 1 and KDFLAG = 1) FORMAT (8X, 3F8.0)		
SAND	Percent sand in soil horizon.	percent
CLAY	Percent clay in soil horizon.	percent
OC	Organic carbon content of soil horizon. This value is also reguired if BDFLAG = 1.	percent
Record TFAT26--ILP, CFLAG FORMAT (2I8)		
ILP	Initial level of pesticide indicator. Signals user to input an initial pesticide storage. ILP = 0, indicates no initial levels input; ILP = 1, indicates initial levels are being input.	--
CFLAG	Conversion flag for initial pesticide level input. CFLAG=0, indicates input in mg kg^{-1}; CFLAG = 1, indicates input in kg ha^{-1}. This flag need not be assigned if ILP = 0.	--
Record TFAT27A--PESTR (Only if ILP = 1) FORMAT (8F8.0)		
PESTR	Initial pesticide level in each compartment (up to NCOM2) as entered from Record TFAT22. Input must be either in mg kg^{-1} or kg ha^{-1}.	--
****************************END OF SOILS DATA******************************		
Record TFAT28--ITEM1, STEP1, LFREQ1, ITEM2, STEP2, LFREQ2, ITEM3, STEP3, LFREQ3 FORMAT (3 (4X, A4 4X, A4, I8)		
ITEM1	Hydrologic output summary indicator. WATR is inserted to call hydrologic summaries. A blank is left for ITEM1 if hydrologic summaries are not desired.	--

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (continued)

Variable	Description	Units
STEP1	Time step of output. Three options are available: DAY for daily, MNTH for monthly, or YEAR for annual output.	--
LFREQ1	Frequency of soil compartment reporting. Example: LFREQ1 = 1, every compartment is output; LFREQ = 5, every fifth compartment is output.	--
ITEM2	Pesticide output summary indicator. PEST is inserted to call pesticide summaries (of mass migration). A blank is inserted for ITEM2 if pesticide summaries are not desired.	--
STEP	Same as STEP1.	--
LFREQ2	Same as LFREQ1.	--
ITEM3	Pesticide concentration profile indicator. CONC is inserted to call pesticide concentration profile summaries. A blank is inserted if concentration profiles are not desired.	--
STEP3	Same as STEP1.	--
LFREQ3	Same as LFREQ1.	--

Record TFAT29--NPLOTS
FORMAT (I8)

NPLOTS	Number of time series to be written to plotting file (maximum of 7).	--

Record TFAT30--PLNAME, MODE, IARG, CONST (Only if NPLOTS is greater than zero)
FORMAT (4X, A4, 4X, A4, I8, F8.0)

PLNAME	Identifier of time series. Possible options are listed in Table 5.6.	--

Table 5.5. INPUT FORMATS FOR THE TERRESTRIAL FATE AND TRANSPORT MODULE (TFAT) (concluded)

Variable	Description	Units
MODE	Plotting mode. Two options are available: TSER provides the time series as output, TCUM provides the cumulative time series.	--
IARG	Argument of variable identified in PLNAME. Example: INFL is specified which corresponds to AINF within the FORTRAN program. AINF is dimensioned from 1 to NCOM2. IARG must be specified to identify the soil compartment (1 to NCOM2) reporting for AINF (IARG is left blank for scalers).	--
CONST	Specifies a constant with which the user can multiply the times series for unit conversion, etc. If left blank a default of 1.0 is used.	

****************************END OF TFAT DATA SET****************************

Table 5.6. VARIABLE DESIGNATIONS FOR TFAT TIME SERIES FILES

Variable Designation (PLNAME)	FORTRAN Variable	Description	Units	Arguments Required (IARG)
Water Storage				
INTS	CINT	Interception storage on canopy	cm	None
SWTR	SW	Soil water storage	cm	1-NCOM2
SNOP	SNOW	Snow pack storage	cm	None
THET	THETN	Soil water content	cm cm^{-1}	1-NCOM2
Water Fluxes				
PRCP	PRECIP	Precipitation	cm day^{-1}	None
SNOF	SNOWFL	Snowfall	cm day^{-1}	None
THRF	THRUFL	Canopy throughfall	cm day^{-1}	None
INFL	AINF	Percolation into each soil compartment	cm day^{-1}	1-NCOM2
RUNF	RUNOF	Runoff depth	cm day^{-1}	None
CEVP	CEVAP	Canopy evaporation	cm day^{-1}	None
SLET	ET	Actual evapotranspiration from each compartment	cm day^{-1}	1-NCOM2
TETD	TDET	Total daily actual evapotranspiration	cm day^{-1}	None
Sediment Flux				
ESLS	SEDL	Event soil loss	Tonnes day^{-1}	None
Pesticide Storages				
EPST	FOLPST	Foliar pesticide storage	g cm^{-2}	None
TPST	PESTR	Total soil pesticide storage in each soil compartment	g cm^{-3}	1-NCOM2
SPST	SPESTR	Dissolved pesticide storage in each soil compartment	g cm^{-3}	1-NCOM2

Table 5.6. VARIABLE DESIGNATIONS FOR TFAT TIME SERIES FILES (continued)

Variable Designation (PLNAME)	FORTRAN Variable	Description	Units	Arguments Required (IARG)
Pesticide Fluxes				
TPAP	TAPP	Total pesticide application	g cm^{-2} day^{-1}	None
FPDL	FPDLOS	Foliar pesticide decay loss	g cm^{-2} day^{-1}	None
WFLX	WOFLUX	Foliar pesticide washoff flux	g cm^{-2} day^{-1}	None
DFLX	DFFLUX	Individual soil compartment pesticide net diffusive flux	g cm^{-2} day^{-1}	1-NCOM2
AFLX	ADFLUX	Pesticide advective flux from each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
DKFX	DKFLUX	Pesticide decay flux in each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
UFLX	UPFLUX	Pesticide uptake flux from each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
RFLX	ROFLUX	Pesticide runoff flux	g cm^{-2} day^{-1}	None
EFLX	ERFLUX	Pesticide erosion flux	g cm^{-2} day^{-1}	None
Pesticide Fluxes				
RZFX	RZFLUX	Net pesticide flux past the maximum root depth	g cm^{-2} day^{-1}	None
TUPX	SUPFLX	Total pesticide uptake flux from entire soil profile	g cm^{-2} day^{-1}	None
TDKF	SDKFLX	Total pesticide decay flux from entire profile	g cm^{-2} day^{-1}	None

Table 5.7. INPUT FORMATS FOR THE PLANT GROWTH (PLTGRN) AND PLANT TRANSLOCATION (PLTRNS) MODULES

Variable	Description	Units
* * * * * * * * * * * * * * * * RECORDS PL1-PL27 * * * * * * * * * * * * * * ARE REPEATED FOR EACH CROP WITHIN EACH HABITAT AND FOR ALL HABITATS		
RECORD PL1 -- ABUFR FORMAT (A5)		
ABUFR	The label 'PLANT' to indicate that a new crop type definition follows.	--
RECORD PL2 -- PHU FORMAT (24X, F10.0)		
PHU	The potential heat units required for the crop to mature.	°C day
RECORD PL3 -- BE FORMAT (24X, F10.0)		
BE	Crop parameter for converting energy to biomass.	kg ha^{-1} $langley^{-1}$
RECORD PL4 -- LAIMX FORMAT (24X, F10.0)		
LAIMX	The maximum leaf area index for the crop.	decimal
RECORD PL5 -- FLAI FORMAT (24X, F10.0)		
FLAI	The fraction of the growing season when leaf area index starts to decline.	decimal
RECORD PL6 -- FGK FORMAT (24X, F10.0)		
FGK	Harvest index - the ratio of total biomass to crop yield.	decimal

Table 5.7. INPUT FORMATS FOR THE PLANT GROWTH (PLTGRN) AND PLANT TRANSLOCATION (PLTRNS) MODULES (continued)

Variable	Description	Units
RECORD PL7 -- RZ FORMAT (24X, F10.0)		
RZ	Potential root depth.	cm
RECORD PL8 -- TBASE FORMAT (24X, F10.0)		
TBASE	Base temperature below which no growth occurs.	°C
RECORD PL9 -- TOPT FORMAT (24X, F10.0)		
TOPT	Optimum growth temperature.	°C
RECORD PL10 -- KHGT FORMAT (24X, F10.0)		
KHGT	Canopy growth rate.	m day^{-1}
RECORD PL11 -- HGTMX FORMAT (24X, F10.0)		
HGTMX	Maximum canopy height.	m
RECORD PL12 -- RW FORMAT (24X, F10.0)		
RW	Reflection coefficient for contaminant transfer from the soil solution to the root.	decimal
RECORD PL13 -- LAMDA FORMAT (24X, F10.0)		
LAMDA	Degradation rate of contaminant within the plant.	day^{-1}

Table 5.7. INPUT FORMATS FOR THE PLANT GROWTH (PLTGRN) AND PLANT TRANSLOCATION (PLTRNS) MODULES (continued)

Variable	Description	Units
RECORD PL14 -- KOW FORMAT (24X, F10.0)		
KOW	Octanol/water partition coefficient for the pesticide.	decimal
RECORD PL15 -- KP FORMAT (24X, F10.0)		
KP	Ratio of the concentration of the contaminant in the nonaqueous phase to the concentration in the aqueous phase within the plant.	$cm^3\ g^{-1}$
RECORD PL16 -- RHONA FORMAT (24X, F10.0)		
RHONA	Ratio of the mass of the nonaqueous aboveground biomass (dry weight) to the total aboveground biomass (wet weight).	$g\ g^{-1}$
RECORD PL17 -- XPOT FORMAT (24X, F10.0)		
XPOT	Potential crop biomass.	$kg\ ha^{-1}$
RECORD PL18 -- XYLD FORMAT (24X, F10.0)		
XYLD	Crop yield.	$kg\ ha^{-1}$
RECORD PL19 -- XRWT FORMAT (24X, F10.0)		
XRWT	Root biomass.	$kg\ ha^{-1}$
RECORD PL20 -- XRWS FORMAT (24X, F10.0)		
XRWS	Mass of sloughed roots.	$kg\ ha^{-1}$

Table 5.7. INPUT FORMATS FOR THE PLANT GROWTH (PLTGRN) AND PLANT TRANSLOCATION (PLTRNS) MODULES (continued)

Variable	Description	Units
RECORD PL21 -- XRWL FORMAT (24X, F10.0)		
XRWL	Mass of live roots.	kg ha^{-1}
RECORD PL22 -- XDPTH FORMAT (24X, F10.0)		
XDPTH	Depth of roots.	cm
RECORD PL23 -- XB FORMAT (24X, F10.0)		
XB	Actual crop biomass.	kg ha^{-1}
RECORD PL24 -- XHGT FORMAT (24X, F10.0)		
XHGT	Crop canopy height.	m
RECORD PL25 -- FB1 FORMAT (24X, F10.0)		
FB1	Dimensionless expression of accummulated thermal time.	decimal
RECORD PL26 -- XCR FORMAT (24X, F10.0)		
XCR	Contaminant concentration within plant roots.	g g^{-1}
RECORD PL27 -- XCAG FORMAT (24X, F10.0)		
XCAG	Contaminant concentration within the aboveground plant biomass.	g g^{-1}

Table 5.8. INPUT FORMATS FOR THE TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM)

Variable	Description	Units
Record APUM1--RLABEL FORMAT (A80)		
RLABEL	A 1 to 80 character run title for the animal data set.	--
****************************RECORDS APUM2-APUM9**************************** ARE REPEATED FOR EACH HABITAT (NHAB Times)		
Record APUM2--NSCOM(IH) FORMAT(I5)		
NSCOM(IH)	Number of soil horizons through which soil animals move in habitat IH (must be less than or equal to the number of TFAT horizons.	--
Records APUM3--NSUB(IH) FORMAT(I5)		
NSUB(IH)	Number of soil animal groups in habitat IH	--
****************************RECORDS APUM4-APUM9**************************** ARE REPEATED FOR EACH SOIL ANIMAL GROUP IN HABITAT IH (NSUB(IH) Times)		
RECORD APUM4--ALABEL(IL) FORMAT(A20)		
ALABEL(IL)	A unique 1 to 20 character label identifying the soil animal IL.	--
RECORD APUM5--PDENS, CO, BCF, KMET, LD10, LD50 FORMAT(6F10.0)		
PDENS	The population density (biomass/unit area) of the animal group corresponding to the label ALABEL in Record APUM4.	g m^{-2}

Table 5.8. INPUT FORMATS FOR THE TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM) (continued)

Variable	Description	Units
CO	The initial concentration of pesticide in the tissues of an organism population.	mg mg^{-1}
BCF	The bioconcentration factor for the animal population in soil.	ratio
KMET	Metabolic degradation rate constant for pesticide in the tissue of the organism population.	$days^{-1}$
LD10	The 10-percentile lethal dosage of pesticide.	mg mg
LD50	The 50-percentile lethal dosage of pesticide.	mg mg
	Note that lethal dosage information is defined on a weight basis of the affected organism, not per weight of ingested food material.	

RECORD APUM6--LD10L, LD10U, LD50L, LD50U
FORMAT(4F10.0)

Variable	Description	Units
LD10L	Lower confidence bound on the LD10	mg mg^{-1}
LD10U	Upper confidence bound on the LD10	mg mg^{-1}
LD50L	Lower confidence bound on the LD50	mg mg^{-1}
LD50U	Upper confidence bound on the LD50	mg mg^{-1}

RECORD APUM7--ICOLD, NMOVE
FORMAT(2I5)

Variable	Description	Units
ICOLD	Soil animal movement flag. =0, animal moves as a population, with the distribution among soil horizons computed from the soil movement transition matrix <0, the animal group is modeled as a population with a steady state distribution among soil horizons.	

Table 5.8. INPUT FORMATS FOR THE TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM) (continued)

Variable	Description	Units
	>0, the animal group moves enmasse by random particle tracking. ICOLD is then the initial soil horizon location.	
NMOVE	The number of times per day that the animal population is redistributed.	days^{-1}
RECORD APUM8--(PMVC(ICO, ICN), I6N = 1, NSCOM(IH) FORMAT(8F10.0) Repeat for each habitat ICO.		
PMVC(ICO, ICN)	The soil horizon movement transition matrix for the animal, containing the probability that the animal will move to each horizon ICN if it is in horizon ICO. Not required for steady-state populations (ICOLD <0).	fraction
RECORD APUM9--(PLHAB(IC), IC = 1, NSCOM(IH)) FORMAT(8F10.0)		
PLHAB(IC)	The fraction of the population contained in each horizon IC. Not required if the animal is modeled by enmasse particle tracking (ICOLD >0).	fraction
RECORD APUM10--NLEVEL FORMAT(I5)		
NLEVEL	The number of higher animal groups (those which prey on other animals and move between habitats).	--

****************************RECORDS APUM11-APUM21****************************
ARE REPEATED FOR EACH HIGHER ANIMAL
(NLEVEL Times)

Table 5.8. INPUT FORMATS FOR THE TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM) (continued)

Variable	Description	Units
RECORD APUM11--ALABEL(IL) FORMAT(A20)		
ALABEL(IL)	A unique 1 to 20 character label identifying the higher animal group IL.	--
RECORD APUM12--MO, CO, UF, KMET, LD10, LD50 FORMAT(6F10.0		
MO	The total biomass of the animal group.	g
CO	The initial concentration of pesticide in the tissues of the organism group.	mg mg^{-1}
UF	The total daily feeding rate for the animal population, per unit body weight.	mg mg^{-1}day^{-1}
KMET	The metabolic degradation rate constant for pesticide in the organism population tissues.	days^{-1}
LD10	The 10 percentile lethal dosage.	mg mg^{-1}
LD50	The 50 percentile lethal dosage.	mg mg^{-1}
RECORD APUM13--LD10L, LD10U, LD50L, LD50U FORMAT(4F10.0)		
LD10L	The lower confidence bound on the LD10.	mg mg^{-1}
LD10U	The upper confidence bound on the LD10.	mg mg^{-1}
LD50L	The lower confidence bound on the LD50.	$^{-1}$
LD50U	The upper confidence bound on the LD50.	mg mg^{-1}
RECORD APUM14--BETA(1), UALPH(1) FORMAT(2F10.0)		
BETA(1)	Preference factor for feeding on soil, as a fraction of the total feeding rate UF on Record APUM12.	fraction
UALPH(1)	Assimilation efficiency for uptake of pesticide from soil.	fraction

Table 5.8. INPUT FORMATS FOR THE TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM) (continued)

Variable	Description	Units
RECORD APUM15--BETA(2), UALPH(2) FORMAT(2F10.0)		
BETA(2)	Preference factor for feeding on plants, as a fraction of the total feeding rate UF.	fraction
UALPH(2)	Assimilation efficiency for uptake of pesticide from plants.	fraction
RECORD APUM16--BETA(3), UALPH(3) FORMAT(2F10.0)		
BETA(3)	Preference factor for feeding on granular pesticide pellets, as a fraction of the total feeding rate UF.	fraction
UALPH(3)	Assimilation efficiency for uptake of pesticide from granules.	fraction
RECORD APUM17--BETA(4), UALPH(4) FORMAT		
BETA(4)	Daily rate of ingestion of ponded water, volume per biomass.	liter mg^{-1} day^{-1}
UALPH(4)	Assimilation efficiency for uptake of pesticide from ponded water.	fraction
RECORD APUM18--BETA(5), UALPH(5) FORMAT(2F10.0)		
BETA(5)	Daily air inhalation rate, volume per unit biomass.	liter mg^{-1} day^{-1}
UALPH(5)	Assimilation efficiency for uptake of pesticide from air.	fraction
RECORD APUM19--IHOLD, NMOVE FORMAT(2I5)		
IHOLD	Habitat movement flag =0, animal moves as a population,	--

Table 5.8. INPUT FORMATS FOR THE TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM) (continued)

Variable	Description	Units
	with the population distribution computed using the habitat transition matrix <0, animal is modeled as a population with a steady-state population distribution. >0, the animal group moves enmasse by random particle tracking. IHOLD is then the initial habitat location number.	
NMOVE	The number of times the animal population is redistributed per day.	days^{-1}

RECORD APUM20--(PMVH(IHO, IHN), IHN = 1, NHAB)
FORMAT(8F10.0)

Variable	Description	Units
PMVH(IHO IHN)	The habitat transition matrix, containing the probability that the animal will move to each habitat IHN if it is in habitat IHO. Record APUM20 is repeated for each habitat IHO, and is not required for steady-state populations (IHOLD <0)	fraction

RECORD APUM21--(PHAB(IH), IH = 1, NHAB)
FORMAT(8F10.0)

Variable	Description	Units
PHAB(IH)	The fraction of the population initially in each habitat IH. Not required for animals moving enmasse by random tracking (IHOLD >0).	fraction

*************************END OF HIGHER ANIMAL DATA************************

Record APUM22--NPRED
FORMAT (I5)

Variable	Description	Units
NPRED	The number of predator-prey pairs to be input in the following records.	--

Table 5.8. INPUT FORMATS FOR THE TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM) (continued)

Variable	Description	Units
****************************RECORDS APUM23-APUM26**************************** ARE REPEATED NPRED TIMES		
Record APUM23--PRED FORMAT (A20)		
PRED	A 1 to 20 character label identifying the predator. PRED must be a predefined higher animal label (ALABEL in Record APUM11).	--
Record APUM24--PREY FORMAT (A20)		
PREY	A 1 to 20 character label identifying the prey. Prey must correspond to a predefined animal label (ALABEL in Records APUM 4 or APUM 11), and may be either a soil animal or a higher animal.	--
Record APUM 25--BETA, FALPH FORMAT (2F10.0)		
BETA	The preference factor for the predator PRED feeding on PREY, as a fraction of the predator's total feeding rate UF on Record APUM12.	fraction
FALPH	The predator's assimilation efficiency for pesticide from the prey.	fraction
Record APUM 26--(PEAT(IH), IH = 1, NHAB) FORMAT (8F10.0)		
PEAT(IH)	The probability that the predator captures the prey in each habitat, given that both animals are in the same habitat.	fraction
***************************END OF PREDATION DATA*****************************		

Table 5.8. INPUT FORMATS FOR THE TERRESTRIAL ANIMAL EXPOSURE MODULE (APUM) (continued)

Variable	Description	Units
Record APUM27--ASTEP FORMAT (A5)		
ASTEP	A character label specifying the time step for printing detailed dosage breakdowns. = 'DAY', daily step = 'MNTH', monthly step = 'YEAR', annual step	
Record APUM28--NPLTS FORMAT (I5)		
NPLTS	The number of time series variables to be written out for plotting and data manipulation.	
******************************REPEAT RECORD A29****************************** NPLTS TIMES		
Record APUM29--TSLBL, TSNAME FORMAT (A5, A20)		
TSLBL	The label for the variable to be plotted: = 'CORG', concentration of pesticide in the organism	(mg mg^{-1})
	= 'DOSE', cumulative pesticide dosage	(mg mg^{-1})
	= 'LD10', 10 percent Lethal dosage	(mg mg^{-1})
	= 'LD50', 50 percent Lethal dosage	(mg mg^{-1})
	= 'LD10L', lower bound on LD10	(mg mg^{-1})
	= 'LD10U', upper bound on LD10	(mg mg^{-1})
	= 'LD50L', lower bound on LD50	(mg mg^{-1})
	= 'LD50U', upper bound on LD50	(mg mg^{-1})
TSNAME	The 1 to 20 character label identifying the animal for which variable TSLBL will be written out (must correspond to a previously defined animal name, Records APUM4 or APUM11)	
******************************END OF APUM DATA******************************		

Table 5.9. INPUT FORMATS FOR THE MONTE CARLO MODULE (MC)

Variable	Description	Units
RECORD MC1 -- TITLE FORMAT (A80)		
TITLE	A 1 to 80 character descriptive title for Monte Carlo Data.	--
RECORD MC2 -- NRUN FORMAT (I5)		
NRUN	The number of Monte Carlo runs to be performed in the simulation.	
**********************END OF SIMULATION CONTROL DATA***********************		
RECORD MC3 -- PNAME, INDX, VAR(1), VAR(2), VAR(3), VAR(4), VAR(5) FORMAT (A20, I10, 5F10.0) Repeat for each Monte Carlo input variable.		
PNAME	The 1 to 20 character name identifying the input parameter to be varied. Currently available parameter names are shown in Table 5.10.	--
INDX	For parameters PNAME which are arrays, the array index to be varied (i.e. the soil horizon number).	
VAR(1)	The mean value for the input variable distribution.	See Table 5.10
VAR(2)	The standard deviation.	See Table 5.10
VAR(3)	The minimum value of the input variable.	See Table 5.10
VAR(4)	The maximum value of the input variable.	See Table 5.10
VAR(5)	A flag indicating the type of distribution to be used in generating values for the input parameter PNAME. Options are: 1 = Normal 2 = Log Normal 3 = Exponential 4 = Uniform 5 = Johnson SB 0 = Constant	--

Table 5.9. INPUT FORMATS FOR THE MONTE CARLO MODULE (MC) (continued)

Variable	Description	Units
RECORD MC4 -- END FORMAT (A3)		
END	The Characters 'END', used to mark the end of input of Record MC3.	
***********************END OF INPUT DISTRIBUTION DATA***********************		
RECORD MC5 -- SNAME (1), INDX, SNAME(2), SNAME(3), NDAYS FORMAT (A20, I10, 2A20, I10) Repeat for each Monte Carlo output variable.		
SNAME (1)	The 1 to 20 character name of the variable to be written out in statistical summaries. Available variable names are shown in Table 5.11.	--
INDX	For variables SNAME(1) which are arrays, the array index to be written out.	--
SNAME(2)	A flag indicating whether a cumulative frequency plot is to be printed for the output variable (indicated by the characters 'CDF').	--
SNAME(3)	A flag indicating that values of the variable are to be written out for each Monte Carlo run (indicated by the characters 'WRITE').	
NDAYS	The number of days in moving average periods (used for statistical output of variables which vary in time).	days
RECORD MC6 -- END FORMAT (A3)		
END	The characters 'END', used to mark the end of Record MC5.	--
****************************END OF OUTPUT DATA******************************		

Table 5.9. INPUT FORMATS FOR THE MONTE CARLO MODULE (MC) (concluded)

Variable	Description	Units
RECORD MC7	-- NAME1, NAME2, CORR FORMAT (2A20, F10.0) Repeat for each pair of correlated variables.	
NAME1	The name of the first correlated variable. NAME1 should correspond to an input PNAME on Record MC3.	--
NAME2	The name of the variable correlated with NAME1. NAME2 should correspond to an input PNAME on Record MC3.	--
CORR	The value of the correlation coefficient between NAME1 and NAME2.	--
RECORD MC8	-- END FORMAT (A3)	
END	The characters 'END', used to mark the end of Record MC7.	--

***************************END OF MONTE CARLO DATA************************

Table 5.10. PNAME LABELS USED TO IDENTIFY MONTE CARLO INPUT VARIABLES

Label	FORTRAN Variable	Description	Units
"SOIL HORIZON DRAIN"	AD(HORIZON)	Soil drainage parameter.	days^{-1}
"SOIL BULK DENSITY"	BD(HORIZON)	Soil bulk density.	$\mathrm{g\ cm}^{-3}$
"PEST DECAY RATE"	DKRATE(HORIZON)	Decay rate of pesticide in soil.	days^{-1}
"PARTITION COEFF/SOIL"	KD(HORIZON)	Partition coefficient between adsorbed and dissolved phase.	$\mathrm{cm}^3\ \mathrm{g}^{-1}$
"SOIL/ROOT REFL COEF"	RW(CROP)	Soil/root reflection coefficient.	--
"PLANT/PEST DECAY"	LAMBA(CROP)	Decay rate of pesticide in plants.	days^{-1}
"OCTANOL/WATER PART"	KOW(CROP)	Octanol water partition coefficient.	$\mathrm{cm}^3\ \mathrm{g}^{-1}$
"ABOVEGROUND WATER"	RHONA(CROP)	Water content in above ground plant material.	fraction
"NONAQ/AQ CONC"	KP(CROP)	Ratio of nonaqueous to aqueous concentration in plants.	--
"BCF"	BCF(ANIMAL)	Bioconcentration factor for soil animals, ratio of organism pesticide concentration to soil pesticide concentration.	--
"FIELD CAPACITY"	THEFC(HORIZON)	Soil water content at field capacity.	$\mathrm{cm}^3\ \mathrm{cm}^{-3}$
"WILTING POINT"	THEWP(HORIZON)	Soil water content of the wilting point.	$\mathrm{cm}^3\ \mathrm{cm}^{-3}$
"FOLIAR DECAY RATE"	PLDKRT	Decay rate constant for foliar pesticide.	days^{-1}
"HENRYS CONSTANT"	KH	Henry's law constant for pesticide vapor.	$\mathrm{cm}^3\ \mathrm{cm}^{-3}$
"APPLICATION RATE"	TAPP(NAPP)	Total mass per unit area of pesticide for the application.	$\mathrm{kg\ ha}^{-1}$
"JULIAN APP. DAY"	IAPDY(NAPP)	The Julian day in which the application occurs.	day

Table 5.10. PNAME LABELS USED TO IDENTIFY MONTE CARLO INPUT VARIABLES (concluded)

Label	FORTRAN Variable	Description	Units
"FALLOW CN"	CN(1,CROP)	SCS Curve number for fallow crop.	--
"CROP CN"	CN(2,CROP)	SCS Curve number for growing crop.	--
"HARVEST CN"	CN(3,CROP)	SCS Curve number for harvested crop.	--
"SOIL PREFERENCE"	UM	Higher animal's preference factor for soil.	fraction
"PLANT PREFERENCE"	UM	Higher animal's preference factor for plants.	fraction
"POND DRINKING RATE"	UM	Rate at which higher animals drink pond water.	liter mg^{-1} day^{-1}
"AIR INHALATION RATE"	UM(ANIMAL,4)	Rate at which higher animals inhale air.	liter mg^{-1} day^{-1}
"GRANULE PREFERENCE"	UM(ANIMAL,5)	Higher animal's preference factor for pesticide granules.	fraction
Name of Prey (variable ALABEL on record APUM4 or APUM11)	BETAF(ANIMAL,PREY)	Preference factor of the higher animal for the indicated prey.	fraction
"METABOLIC DEGRAD"	KMET(ANIMAL)	Metabolic degradation rate for pesticide in animal.	$days^{-1}$
"TOTAL FEEDING RATE"	UF(ANIMAL)	Total feeding rate for animal, as fraction of body weight per day (for higher animals only).	mg $mg^{-1}day^{-1}$

NOTE: Variables dimensioned by HORIZON require the user to input the soil horizon number for INDX on Record MC3. Variables dimensioned by CROP require the crop number, while variables dimensioned by ANIMAL require the animal number. Variables dimensioned by NAPP require the user to input the application number. Crops and animals are numbered in the order in which they are input on the TFAT and APUM data files.

Table 5.11. SNAME LABELS USED TO IDENTIFY MONTE CARLO OUTPUT VARIABLES

Label	FORTRAN Variable	Description	Units
"SOIL HORIZON DRAIN"	AD(HORIZON)	Soil drainage parameter.	days^{-1}
"SOIL BULK DENSITY"	BD(HORIZON)	Soil bulk density.	g cm^{-3}
"PEST DECAY RATE"	DKRATE(HORIZON)	Decay rate of pesticide in soil.	days^{-1}
"PARTITION COEFF/SOIL"	KD(HORIZON)	Partition coefficient between adsorbed and dissolved phase.	cm^3 g^{-1}
"SOIL/ROOT REFL COEF"	RW(CROP)	Soil/root reflection coefficient.	--
"PLANT/PEST DECAY"	LAMDA(CROP)	Decay rate of pesticide in plants.	days^{-1}
"OCTANOL/WATER PART"	KOW(CROP)	Octanol water partition coefficient.	cm^3 g^{-1}
"ABOVEGROUND WATER"	RHONA(CROP)	Water content in aboveground plant material.	fraction
"NONAQ/AQ CONC"	KP(CROP)	Ratio of nonaqueous to aqueous concentration in plants.	--
"BCF"	BCF(ANIMAL)	Bioconcentration factor for soil animals, ratio of organism pesticide concentration to soil pesticide concentration.	--
"METABOLIC DEGRAD"	KMET(ANIMAL)	Metabolic degradation rate for pesticide in animals.	days^{-1}
"FIELD CAPACITY"	THEFC(HORIZON)	Soil water content at field capacity.	cm^3 cm^{-3}
"WILTING POINT"	THEWP(HORIZON)	Soil water content at the wilting point.	cm^3 cm^{-3}

Table 5.11. SNAME LABELS USED TO IDENTIFY MONTE CARLO OUTPUT VARIABLES (continued)

Label	FORTRAN Variable	Description	Units
"FOLIAR DECAY RATE"	PLDKRT	Decay rate constant for foliar pesticide.	days^{-1}
"HENRYS CONSTANT"	KH	Henry's law constant for pesticide vapor.	$\text{cm}^3\ \text{cm}^{-3}$
"APPLICATION RATE"	TAPP(NAPP)	Total mass per unit area of pesticide for the application.	kg ha^{-1}
"JULIAN APP. DAY"	IAPDY(NAPP)	The Julian day in which the application occurs.	day
"FALLOW CN"	CN(1,CROP)	SCS Curve number for fallow crop.	--
"CROP CN"	CN(2,CROP)	SCS Curve number for growing crop.	--
"HARVEST CN"	CN(3,CROP)	SCS Curve number for harvested crop.	--
"SOIL PREFERENCE"	UM	Higher animal's preference factor for soil.	fraction
"PLANT PREFERENCE"	UM	Higher animal's preference factor for plants.	fraction
"POND DRINKING RATE"	UM	Rate at which higher animals drink pond water.	$\text{liter mg}^{-1}\ \text{day}^{-1}$
"AIR INHALATION RATE"	UM(ANIMAL,4)	Rate at which higher animals inhale air.	$\text{liter mg}^{-1}\ \text{day}^{-1}$
"GRANULE PREFERENCE"	UM(ANIMAL,5)	Higher animals preference factor for pesticide granules.	fraction

Table 5.11. SNAME LABELS USED TO IDENTIFY MONTE CARLO OUTPUT VARIABLES (concluded)

Label	FORTRAN Variable	Description	Units
Name of Prey (variable ALABEL on record APUM4 or APUM11)	BETAF(ANIMAL,PREY)	Preference factor of the higher animal for the indicated prey.	fraction
"TOTAL FEEDING RATE"	UF(ANIMAL)	Total feeding rate for animal, as fraction of body weight per day (for higher animals only).	mg mg^{-1} day^{-1}
"FOLIAR PESTICIDE"	FOLPST	Pesticide mass on plant foliage.	kg ha^{-1}
SOIL PESTICIDE"	PESTR(LAYER)	Pesticide concentration in soil layers. Requires soil layer number for INDX on Record MC3.	kg ha^{-1}
"ATMOSPHERIC PEST"	CCAN	Atmospheric pesticide concentration.	g cm^{-3}
"ROOT CONC"	XCR	Pesticide concentration in roots.	g g^{-1}
"ABOVEGROUND CONC"	XCAG	Pesticide concentration in aboveground plants.	g g^{-1}
"ORG PEST CONC/ANIM"	CO(ANIMAL)	Concentration of pesticide in animals.	g g^{-1}
"PESTICIDE DOSAGE"	DOSE(ANIMAL)	Daily pesticide dosage for animals.	g g^{-1}

NOTE: Variables dimensional by HORIZON require the user to input the soil horizon number for INDX on Record MC3. Variables dimensional by CROP require the crop number, while variables dimensional by ANIMAL require the animal number. Crops and animals are numbered in the order in which they are input on the TFAT and APUM data files.

Variables dimensioned by NAPP require the user to input the application number.

SECTION 6

PARAMETER ESTIMATION

6.1 INTRODUCTION

In this section, guidance for estimating model parameters is given. Not all parameters are mentioned. Values of those parameters which are simply switches for options are described in sufficient detail in Section 5. Similarly, parameters which specify options for output, etc. (i.e., plotting file variable name designations) are dealt with only in Section 5. Those parameters which require special knowledge to estimate are included in this section. These include parameters such as dispersion coefficients, adsorption coefficients, and other rates and constants. Guidance for some parameters is unavailable. In general, the user is given specific guidance, where it is possible, with references to documents which may contain additional information. Parameter distribution information, as well as information on mean values, is given, where possible, for use in Monte Carlo simulation. The guidance is arranged, according to computational module, in the following sequence:

- FSCBG
- GRDDEP
- TFAT
- PLTGRN
- PLTRNS
- APUM

6.2 FSCBG PARAMETERS

The FSCBG model can be used to simulate either aerial applications or ground spray events. In the form installed in TEEAM, FSCBG should be relatively easy to use. Many of the parameters have default values and, unless specific information is available to the contrary, the user is encouraged to take advantage of these values. Default values are indicated in Table 5.2a in Section 5. Values for parameters of aerial applications which the user may want to estimate for his particular application are covered first.

6.2.1 Aerial Spray Application

The aerial application module requires the following groups of parameters:

- Meteorological
- Source input and
- Spray distribution

6.2.1.1 Meteorological Inputs--

A number of meteorological inputs are required for the FSCBG model. However, as stated above, only a few need be entered by the user. Guidance available to the authors for estimating these parameters is given below:

SIGAD and SIGEP standard deviation of the wind azimuth angle and standard deviation of wind elevation angle--These values are set internally for various atmospheric stability regions. Stability regions are derived from the Richardson number computed in TFAT. They are not required as user inputs.

HM--surface mixing layer height--The mixing layer height is that height to which a parcel of air at the surface, after heating, will continue to rise until its temperature equals the local atmospheric temperature. The extent to which this mixing takes place varies diurnally and from season to season. Typical values which have been used include those found in Table 6-1 for six different meteorological regimes.

WSOCAN--wind speed above the canopy--This parameter is no longer required by FSCBG as a TEEAM module. Daily wind speeds are read from the meteorological file.

THETA--wind direction--The user should enter a typical value of wind direction for the location of concern.

RELHMO--relative humidity above the canopy--A typical value for the site should be used. It is entered as a percent and should be obtainable from local meteorological information.

AIRPRS--barometric pressure--The user should use a value typical for the location of the ecosystem.

AIRTPO--air temperature above the canopy--This is no longer required as an input parameter when FSCBG is used as a TEEAM module as it is read daily from the meteorological file.

TABLE 6-1. FSCBG PARAMETER SPECIFICATIONS FOR FOUR METEOROLOGICAL REGIMES

Location	Time of Morning	Wind Speed mi/h	Wind Speed m/s	H_m (m)	$\sigma_A\{\tau_o=600s\}$[3] (deg)	σ_E (deg)
Marine	Early	1.5	0.67	115	6.5	2.2 [1]
	Early	3.0	1.34	115	6.5	2.2
	Late	3.0	1.34	315	15.0	5.0
	Late	6.0	2.68	415	10.0	3.3
Florida	Early	4.5	2.00	100	5.0	1.67[2]
	Late	11.0	5.00	00	8.0	2.67

[1] Dumbauld et al. 1980

[2] Rafferty and Dumbauld 1980

[3] GA and GE refer to SIGAD and SIGEP referred to in this section.

6.2.1.2 Source Inputs--

Q--source strength--The source strength Q (gm^{-1}) can be calculated by knowing the desired application rate liquid density and swath width as follows:

$$Q(g\ m^{-1}) = 0.935\ (DENLIQ)\ (SWATH)\ (Q(gal\ ac^{-1}) \qquad (6\text{-}1)$$

in which

$Q(g\ m^{-1})$ is the application rate in $g\ m^{-1}$
DENLIQ is the density of the formulation ($g\ cm^{-3}$)
SWATH is the swath width (m)
Q is the application rate ($gal\ ac^{-1}$)
0.935 is a conversion factor

If Q is known in Kg/ha or lb/ac, the $Q(g\ m^{-1})$ can be calculated by

$$Q\ (g\ m^{-1}) = 0.1\ (SWATH)\ Q(Kgha^{-1}) \text{ or} \qquad (6\text{-}2)$$

$$Q\ (g\ m^{-1}) = 0.112\ (SWATH)\ Q(lb\ ac^{-1}) \qquad (6\text{-}3)$$

HGTCFT--spray release height--The spray release height depends upon the aircraft type and the canopy height of the crop being sprayed. Typical release heights are 1.5 to 6 m for row crops and 15 to 20 m for forests.

ARCWGT--aircraft weight--Aircraft weight varies according to the model. Table 6-2 gives aircraft model specific parameters for a number of aircraft.

WNGSPN--aircraft (or rotor diameter) wingspan--See Table 6-2.

ARCRSP--aircraft speed--See Table 6-2.

SIGXYZ--source dimension--This source dimension is typically estimated from the visible width of the spray cloud behind the aircraft. Under the assumption that the spray cloud is Gaussian in shape and that the visible edge of the cloud represents the point at which the concentration is one-tenth of that of the cloud centroid, the source dimension is found by dividing the visible width by 4.3. A typical value for the visible width is 1.5 times the wingspan (Dumbauld et al. 1980). Thus,

$$SIGXYZ = 1.5\ WNGSPN/4.3 \qquad (6\text{-}4)$$

Input values used for a Bell G-3 helicopter were 15.1 to 18.6 m (Dumbauld et al. 1977). However, based on equation 6-4, values would appear to be much smaller.

WAKVEL--wake settling velocity--The wake settling velocity is computed according to

$$W = \frac{8g\ W_a\ (10^{-3})}{\pi^3\ P_a\ b^2\ V_a} \qquad (6\text{-}5)$$

in which

W_a is the weight of the aircraft (ARCWGT) (kg)
g is gravitational acceleration (9.8 m s^{-1})
P_a is the air density (g cm^{-3})
b is the aircraft wingspan or rotor diameter (WNGSPN) (m) and
V_a is the aircraft speed (ARCRSP) (m s^{-1})

DECAY--coefficient of exponential decay of sprayed material--Unless the user has specific information concerning the decay of the material during the spray event, this coefficient should be set to zero. Unless the chemical decays rapidly by photolysis, it is doubtful that significant decay occurs during the relatively short residence time of the chemical in the air.

TABLE 6-2. AIRCRAFT SPECIFIC MODEL PARAMETERS[1]

Aircraft	Weight (Kg)	Wingspan or Rotor Diameter (m)	Typical Working Speed (ms^{-1})
Ayres			
52R-600 Thrush	3140	13	50
52R Turbo Thrush	3900	13	60
52R-1820 Bull Thrush	4550	13	60
Air Tractor			
AT-400	3545	13.5	64
AT-301	3320	13.5	62
Bell			
Jet Ranger III (206B)	1455	10	10-25
G-3	1050	11.3	22[2]
Cessna			
Ag Husky	2000	12.6	53
Ag Truck	1910	12.6	50
Bellanca (formerly Eagle)			
Eagle DW-1	2410	16.5	44
Melex (Pezetal)			
M18 Dromander	4200	17.7	70
Hiller			
WH-12E	1410	10.5	26
Erstrom			
280F	1180	9.6	35
F-28F	1180	9.6	35
Schweizer/Hughes			
300C	930	--	11
500C	1100	7.7	11
Schweizer/Ag Cat			
G-164B	3190	12.8	50
G-164B Turbine	3190	12.8	57
Piper			
Brave 400	2180	11.6	55
Weatherly			
620	2680	11.6	55
620 TP	2770	12.3	57

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[1] Source: Agricultural Aviation 1984, except where otherwise indicated

[2] Source: Dumbauld, Rafferty and Bjorklund 1977

6.2.1.3 Spray Distribution--

The two principal parameters which the user must enter are the drop size distribution and mass percentage of the material in each drop size fraction. A typical distribution is shown in Table 6-3. Upper and lower drop size limits (DRPUPR and DRPLWR) are shown in the first two columns. The fraction of material in each drop size fraction (PCTMAT) is given in the third column. The drop size distribution will obviously depend upon the nozzle size. Table 6-4 from Akesson and Yates (1976) shows the drop size range and typical uses for various nozzle sizes. Table 6-5 from the same reference gives drop size distribution and cumulative percent by volume for each size range.

TABLE 6-3. TYPICAL FSCBG SPRAY DROP SIZE DISTRIBUTION PARAMETERS

Drop Upper Limit (m) DRPUPR	Drop Lower Limit (m) DRPLWR	Fraction of Material In Drop-Size Category PCTMAT
1420	1020	0.01
1020	840	0.02
840	742	0.03
742	667	0.04
667	577	0.10
577	514	0.10
514	456	0.10
456	351	0.20
351	302	0.10
302	253	0.10
253	200	0.10
200	169	0.04
169	135	0.03
135	100	0.02
100	51.6	0.009
51.6	20.0	0.001

Source: Dumbauld et al. 1980

TABLE 6-4. SPRAY DROP SIZE RANGE, APPROXIMATE RECOVERY RATE, AND RECOMMENDED USE OF VARIOUS SPRAY NOZZLE TYPES

Spray Size or Type and Description of Spray System	Typical Nozzles and Pressure Ranges	Drop Size Range[2] (Microns µm vmd)	Estimated Deposit in 1000 Feet[3] (Percent)	Use
Coarse aerosols Cone and fan nozzles, and rotary atomizers	80005 down D2-13 down (200 to 300 lb/in^2)	less than 125	less than 125	Aerosol applications, in vector control and control of forest insects and agricultural pathogens; used at low volume rates, primarily for adulticiding
Fine sprays Cone and fan nozzles, and rotary atomizers	80005 down D6-45 down (50 to 100 lb/in^2)	100 to 300	40 to 80	Forest pesticide chemicals, in large-area vector control, at low dosages of chemicals with low toxicity and rapid degradation; also useful for agricultural insect pathogens
Medium sprays Cone and fan nozzles and rotary atomizers	D6-46 down (30 to 50 lb/in^2)	300 to 400	70 to 90	All low-toxicity agricultural chemicals where good coverage is necessary
Coarse sprays Cone and fan nozzles, spray additives	D6-46 back (30 to 50 lb/in^2)	400 to 600 with additives up to 2000	85 to 98	Toxic pesticides of restricted classification, when thorough plant coverage is not essential
Sprays with minimum drift Jet nozzles and spray additives	D4 to D8 down at less than 60 mph; back at over 60 mph (30 to 50 lb/in)	800 to 1000 with additives up to 5000	95 to 98	All toxic, restricted-class herbicides such as phenoxy-acids and others, within limitations such as growing season and location near susceptible crops
Sprays with maximum drift control Low-turbulence nozzles	Microfoil (less than 60 mph airstream)[4]	800 to 1000	90 or more	Restricted nonvolatile herbicides, phenoxy-acids and others in the area of susceptible crops, subject to limitations of growing season and type of crop

[1] Spraying Systems Co. nozzles; position on aircraft boom is indicated as "down" or with the airstream.
[2] Determined with water base sprays; oils would give smaller drops.
[3] 1000 feet downwind; wind velocity 3 to 5 mph, neutral temperature gradient; material released under 10 feet height.
[4] In drift tests, drift residue levels at 500 feet downwind for Microfoil were one-fourth those for D4 to D8 jets.

Source: Akesson and Yates (1976).

TABLE 6-5. DROP SIZE DISTRIBUTION OF AEROSOLS AND SPRAYS, CUMULATIVE PERCENT BY VOLUME[1]

Drop Size (μm)	Fine Aerosols	Coarse Aerosols	Fine Sprays	Medium Sprays	Coarse Sprays	Very Coarse Sprays
	Cumulative Percent					
1-5	5	0.1				
5-10	45	0.4	0.1			
11	50					
10-15	77	2.0				
15-20	97		2.0			
20-40	100	12.0		0.1		
40-60		35.0	5.0	2.0	0.01	0.001
60-80						
86		50.0				
80-100		59.0	15.8	6.0	0.1	
100-120						
120-140					0.4	0.1
130			50.0			
140-180		100.0				
180-200			81.0	17.0	3.0	
200-220						
220-240					7.0	5.0
240-260						
260-280						
280-300			100.00	46.0	14.0	
278				50.0		
300-350					24.0	
350-400					36.0	
400-450					46.0	
460					50.0	
450-500				92.0	55.0	
500-600					74.0	25.0
600-700					88.0	
700-800					96.0	
900						50.0
800-1000				100.0	100.0	100.0

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[1] The volume median diameter (underscored) is that size of drop which divides the total volume of drops found exactly in half; that is, 50 percent of the volume is in drops above that size and 50 percent below.

Source: Akesson and Yates (1976).

ISW (2)--evaporation model option--The user is encouraged to use ISW (2) = 0, with which no evaporation will be assumed. If the use of the evaporation calculations are essential the user is encouraged to use ISW (2) = 1. In this mode, the model performs drop evaporation computations. The user should avoid option ISW (2) = 2 unless he has very specific data about drop evaporation in the spray over time.

6.2.2 Ground Spray Applications

The FSCBG (Version 1.0) computer program is not designed for direct modeling of ground vehicle spray releases. However, the program can be used to model some types of ground vehicle spray releases if care is used in selecting the model inputs. The FSCBG (Version 1.0) program assumes spray material is released along a line from a moving vehicle and after a short period of time material falls to the surface subject due to meteorological and gravitational forces. During ground vehicle spray operations spray material is often directed lateral to the vehicle movement or is sprayed to the rear of the vehicle. The FSCBG (Version 1.0) program does not account for the effects on drop material due to the forced spray trajectory. Therefore, to model these applications, parameters associated with the spray must be modified to account for the displacement of the drops, the distance over which they are subject to evaporation, and the distance over which they are subject to meteorological forces. Further, the FSCBG (Version 1.0) code cannot model direct impaction of material due to a forced spray. FSCBG (Version 1.0) input parameters that require special attention for ground vehicle spray releases are given below for two general modes of application. Obviously, for these applications, the aircraft wake model should be turned off.

6.2.2.1 Spray Perpendicular to Vehicle Movement--

The first mode of application assumes nozzles are mounted on a spray boom perpendicular to the movement of the vehicle and spray material is directed to the back of the vehicle in the plane of travel. If the spray nozzles are directed down, FSCBG (Version 1.0) should not be used, because the program cannot account for impaction due to the forced spray.

NSOURC--This parameter specifies the number of spray lines in the direction of vehicle travel. Ideally, the number of lines is given by the number of nozzles mounted on the boom. However, if there is sufficient overlap of the spray from adjacent nozzles, a single line can be used. Sufficient overlap requires that the width (diameter) of the spray plume is roughly twice the distance between nozzles at or before the spray material reaches the apex of the spray trajectory.

Q--This parameter specifies the rate of application of the spray mixture in grams per meter of travel. If each nozzle is being modeled as a single line, Q is the amount of material from a single nozzle. If nozzles are grouped into a single line, Q is the sum of the material from the number of nozzles used.

SIGXYZ--This parameter specifies the standard deviation of the spray material distribution. If each nozzle is being modeled as a single line, this quantity is approximated by the width (diameter) of the spray plume at the apex of the spray trajectory divided by 4.3 However, if nozzles are grouped into a single line, the width is the distance from the outer edge of the first nozzle plume to the outer edge of the last nozzle plume.

XLRZ--This parameter is greater than zero and is approximated by the horizontal distance to the value specified by SIGXYZ above.

DRPUPR, DRPLWR--These parameters give the upper and lower statistical bounds of the drop diameter for each drop size category. These values are obtained from the manufacturer of the spray nozzle, known distributions, or published studies such as Measurement of Drop Size Frequency from Nozzles Used for Aerial Applications of Pesticides in Forests (USDA Forest Service October 1984). However, information obtained from aircraft nozzle studies should be used with caution because of the great differences between ground vehicle and aircraft spray, such as the much greater speed of the aircraft. Values must be entered in descending order of size. Multiple categories of the same size, gaps between size categories or a single size category will generally produce erroneous results. The minimum drop diameter that can be entered is 5 micrometers.

HGTCFT--This parameter specifies the effective release height of the spray material. The FSCBG (Version 1.0) program does not contain the physics required to directly model the forced spray trajectory. Because evaporation, some dispersion, and trajectory modification due to wind speed and direction occurs prior to the apex of the spray trajectory, the specific height to use is ill-defined. The height to use is somewhere between the distance along the trajectory from the apex to the surface and the entire length of the trajectory. Generally, the height would be that distance over which meteorological forces dominate the spray plume.

DX, DY--These parameters specify the start and end point of each spray line. If a single line is being modeled, use the center of the vehicle. If each nozzle represents a source, use the relative location of each nozzle.

6.2.2.2 Spray Parallel to Vehicle Movement--

The second mode of application assumes nozzles are mounted on a spray boom parallel to the movement of the vehicle and spray material is directed perpendicular to the vehicle plane of travel. If spray nozzles are directed down, FSCBG (Version 1.0) should not be used, because the program cannot account for impaction due to the forced spray.

NSOURC--This parameter specifies the number of spray lines in the direction of vehicle travel. This parameter in this case would generally be one unless multiple passes were made by the vehicle. This assumes that each drop size category travels the same distance along the spray trajectory. In actual practice, however, the larger drops will travel further due to momentum effects. If the distance of travel for specific groups of drop size categories is known, the problem could be broken into multiple FSCBG program runs, one for each group of categories and the results manually summed over the number of runs used.

Q--This parameter specifies the rate of application of the spray mixture in grams per meter of travel. This value would be the sum of the quantity sprayed by all nozzles.

SIGXYZ--This parameter specifies the standard deviation of the spray material distribution. This quantity is approximated by the width (diameter) of the spray plume from a single nozzle at the apex of the spray trajectory divided by 4.3. If multiple runs are made over groups of drop size categories, the value used is determined for the specific drop size categories.

XLRZ--This parameter is greater than zero and approximated by the horizontal distance to the value specified by SIGXYZ above.

DRPUPR, DRPLWR--These parameters give the upper and lower statistical bounds of the drop diameter for each drop size category. These values are obtained from the manufacturer of the spray nozzle, known distributions, or published studies such as Measurement of Drop Size Frequency from Nozzles Used for Aerial Applications of Pesticides in Forests, USDA Forest Service, October 1984. However, information obtained from aircraft nozzle studies should be used with caution because of the great differences between ground vehicle and aircraft spray, such as the much greater speed of the aircraft. Values must be entered in descending order of size. Multiple categories of the same size, gaps between size categories or a single size category will generally produce erroneous results. If multiple program runs are being made over groups of drop size categories, the sum of the mass fractions (PCTMAT) must equal one over all runs. The minimum drop diameter is 5 micrometers.

HGTCFT--This parameter specifies the effective release height of the spray material. The FSCBG (Version 1.0) program does not contain the physics required to directly model the forced spray trajectory. Because evaporation, some dispersion and trajectory modification due to wind speed and direction occurs prior to the apex of the spray trajectory, the specific height to use is ill-defined. The height to use is somewhere between the distance along the trajectory from the apex to the surface and the entire length of the trajectory. Generally, the height would be that distance over which meteorological forces dominate the spray plume.

DX, DY--These parameters specify the start and end points of each spray line. The spray material is sprayed out along a line parallel to the movement of the venicle. In this case, use the best estimate, based on the force and angle of the spray and meteorological conditions.

6.3 GRDDEP PARAMETERS

The GRDDEP module provides a linkage between the FSCBG model, whose output is defined on a two-dimensional grid, to TFAT habitats, which cannot make use of spatially distributed information. The function of GRDDEP is to compute average deposition values and map spray deposition information into TFAT habitats. It requires inputs which map TFAT habitats onto the FSCBG grid. Habitats may only be quadrilateral in shape. The important parameters for the user's consideration are described below.

6.3.1 XSW, YSW, XNE, YNE--Habitat Coordinates

The user enters the southwest (x,y) coordinates and northeast (x,y) coordinates of each habitat. Note that the FSCBG grid is oriented north-south, although the swath lines may be oriented at any angle. The x coordinates must increase from west to east and the y coordinates must increase from south to north. GRDDEP uses these coordinates to compute habitat area for deposition averaging calculations. The user should exercise caution that these areas match the habitat area entered in the TFAT input stream. (The program does an internal check to insure that these areas match within ±10%. The habitat area is left in the TFAT input stream in the case that FSCBG and GRDDEP are not used.) GRDDEP computes this area by finding the FSCBG grid points which lie within the specified habitat quadrilateral, and then summing the areas assigned to each grid point. As these areas are computed by multiplying the X axis increment by the Y axis increment, the user should locate XSW, YSW, XNE and YNE at the centroid of an area defined by FSCBG grid points. By doing this, the area defined by the coordinates, the area computed by GRDDEP and the habitat area read for TFAT habitats will be equal.

In GRDDEP, the user also specifies the number of spray applications and how the deposited spray will be distributed between soil and canopy, and within the canopy. (The simulation results of distribution within the canopy are not used by TEEAM, however, the parameters to simulate this effect must be entered.) The user is directed to the description of these parameters in Section 6.4.1.3.

6.4 TFAT PARAMETERS

With a few exceptions, the TFAT module has the same input formats and parameter requirements as PRZM (Carsel et al. 1984). This section contains guidance for the original PRZM parameters (6.4.1) as well as additional parameters required by TFAT. New groups of parameters include:

- Infiltration and ponding (6.4.2)
- Pond chemistry (6.4.3)
- Volatilization (6.4.4)
- Granular Pesticide Fate (6.4.5)

Note that some of the original PRZM parameters (e.g., SFAC, PFAC, ANETD, etc.) are read in the TEEAM Execution Supervisor input file. These parameters are discussed here however.

6.4.1 Original PRZM Parameters

TFAT relates pesticide fate in the upper soil to temporal variations in hydrologic, agronomic, and pesticide chemical factors. A minimum of generally accessible input is required for successful use of TFAT. The module does utilize some parameters, however, that users may find difficult to obtain or calculate. The following section describes these parameters and provides detailed procedures for estimating or obtaining the required values. Parameters appear in the same general order that they appear in the input file. Options are available in the program to directly estimate several parameters (THEFC, THEWP, BD, and KD) when related information is supplied by the user.

6.4.1.2 Hydrology Parameters--

NPTIME--number of time steps for ponding computations--A value of 24 hours is recommended.

SFAC and PFAC--snow factor and pan factor--When the mean air temperature falls below 0.0 °C, any precipitation that falls is considered to be in the form of snow. When the mean air temperature is above 0.0 °C, however, the snow accumulation is decreased by a snowmelt factor, SFAC.

The mean air temperature is read from the meteorological file and provides a value for (T). The snowmelt factor, SFAC, for site-specific analyses can be obtained from Linsley et al. (1975). The mid-range of their values is 0.46 cm day^{-1}. The calculated snowmelt is used to estimate the antecedent moisture condition and subsequently the runoff caused by the snowmelt. The snow factor would be applicable only to those areas in which temperatures are conducive to snowfall and accumulation.

The pan factor (PFAC) is a dimensionless number used to convert daily pan evaporation to daily potential ET. The pan factor generally ranges between (0.60-0.80). Figure 6.1 illustrates typical pan factors in specific regions of the United States.

ANETD--soil evaporation moisture loss during fallow, dormant periods-- The soil water balance model considers both soil evaporation and plant transpiration losses and updates the depth of root extraction. The total ET demand is subtracted sequentially in a linearly weighted manner from each layer until a minimum moisture level (wilting point) is reached within each layer. Evaporation is initially assumed to occur in the top 10 cm of the soil profile with the remaining demand, crop transpiration, occurring from compartments below the 10-cm zone and down to the maximum depth of rooting. These assumptions allow simulation of reduced levels of ET during fallow, dormant periods and increased levels during active plant growth. Values for (ANETD) used to estimate soil evaporation losses are provided in Figure 6.2.

The values for ANETD in Figure 6.2 are only applicable for soil hydraulics option 1, the free drainage model, and would not be appropriate for use with hydraulics option 2, the limited drainage model. The limited drainage model allows more available soil water and, hence, more ET extraction. If drainage option 2 is selected, it is recommended that ANETD be set to equal 10 cm. Calibration may be required if results are not consistent with local water balance data.

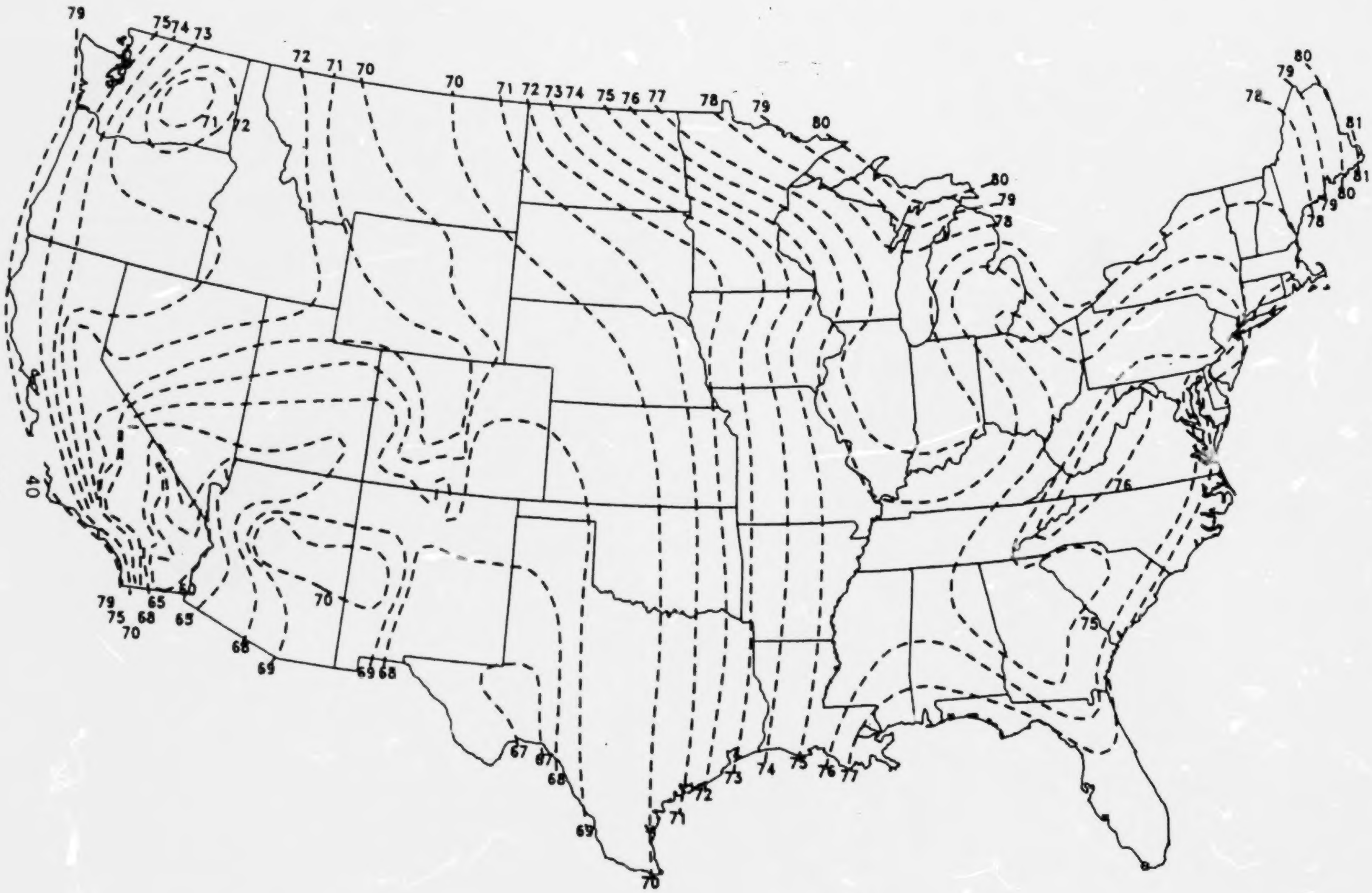
DT--average day time hours for a day in each month--The values of DT are used to calculate total potential ET using Hamon's Formula if daily pan evaporation data do not exist. Values of DT for latitudes 24 - 50° north of the equator are provided in Table 6-6.

Values for DT are determined by:

Step 1. Finding the approximate degree latitude north of the equator for the agricultural use site under consideration.

Step 2. Inputting the 12 monthly numbers under the degree latitude column into the parameter file (e.g., 42° north latitude).

9.4, 10.4, 11.7, 13.1, 14.3, 14.9, 14.6, 14.0, 12.3, 10.9, 9.7, 9.0


79
75 74 73
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78 79 80
78 79 80 81
80 79 78
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65 68
60 65
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71 72 73 74 75 76 77

Figure 6.1 Pan evaporation correction factors (from U.S. Weather Bureau).

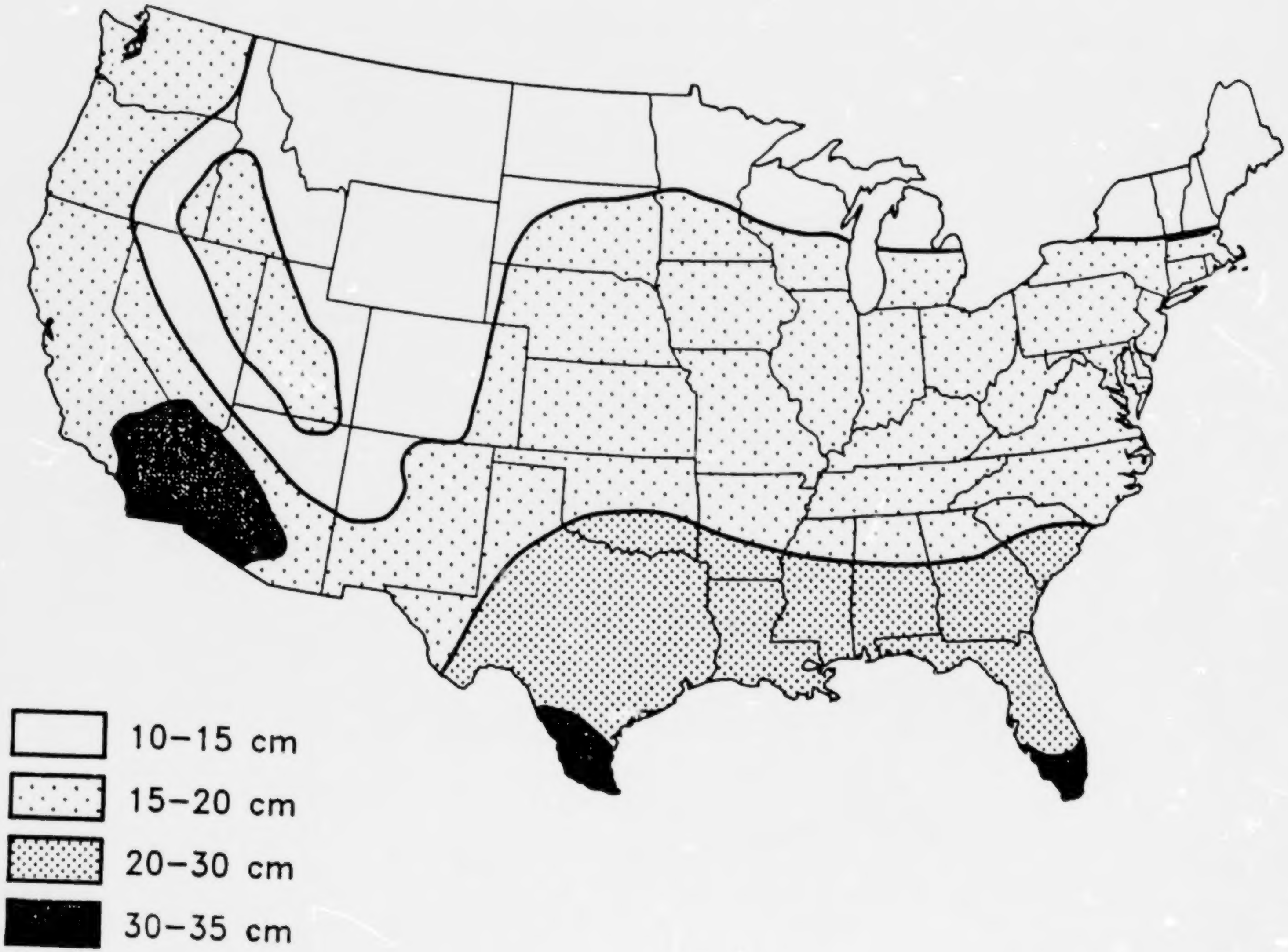
10–15 cm
15–20 cm
20–30 cm
30–35 cm

Figure 6.2 Diagram for estimating soil evaporation loss.

TABLE 6-6. ACTUAL DAYTIME HOURS FOR LATITUDES 24° TO 50° NORTH OF EQUATOR

Month	Latitudes (in degrees north of Equator)													
	24	26	28	30	32	34	36	38	40	42	44	46	48	50
Jan.	10.7	10.6	10.5	10.3	10.2	10.0	9.9	9.7	10.0	9.4	9.2	8.9	8.7	8.4
Feb.	11.2	11.1	11.1	11.0	10.9	10.8	10.7	10.6	10.5	10.4	10.3	10.2	10.0	9.9
Mar.	11.9	11.9	11.9	13.1	11.9	11.8	11.8	11.8	11.8	11.7	11.7	11.7	11.7	11.7
Apr.	12.6	12.6	12.7	12.7	12.8	12.8	12.9	13.0	13.1	13.1	12.8	13.3	13.4	13.5
May	13.1	13.7	13.4	13.5	13.7	13.7	13.9	14.1	14.2	14.3	15.0	14.7	14.9	15.1
June	13.4	13.6	13.8	13.9	14.0	14.2	14.4	14.5	14.7	14.9	15.2	15.4	15.6	15.6
July	13.3	13.4	13.5	13.7	13.9	14.0	14.1	14.3	14.4	14.6	15.0	15.0	15.3	15.5
Aug	13.7	13.3	13.4	13.5	13.5	13.6	13.7	13.8	13.9	14.0	14.2	14.3	14.4	14.6
Sept.	12.1	12.1	12.1	12.2	12.2	12.2	12.2	12.2	12.2	12.3	12.3	12.3	12.3	12.3
Oct.	11.4	11.4	11.2	11.2	11.2	11.2	11.1	11.0	11.0	10.9	10.8	10.7	10.6	10.5
Nov.	10.8	10.7	10.6	10.5	10.4	10.5	10.1	10.0	9.8	9.7	9.5	9.3	9.6	8.9
Dec.	10.5	10.4	10.3	10.1	10.0	9.8	9.6	9.4	9.2	9.0	8.8	8.5	8.3	8.0

Source: Criddle, W.D. (1958).

USLEK, USLELS, USLEP, USLEC soil erosion--Universal Soil Loss Equation--The role of erosion on pesticide loss decreases with decreasing chemical affinity for soil. The total mass of pesticide loss by this means for most highly soluble pesticides will be quite small. If the apparent distribution coefficient is less or equal to 5.0, erosion can be neglected (i.e., the erosion flag ERFLAG can be set to zero). For a compound having a distribution coefficient greater than 5.0, erosion losses (and subsequent pesticide loss) should be estimated and the erosion flag set (to one) accordingly.

Soil characteristics, climatic conditions, agronomic practices and topography contribute to the potential erosion rate from a field. During an erosion-producing runoff event, soil particles and aggregates are carried across the field. These aggregates consist of coarse, medium, and fine particles, with the fine particles (sediment) carried the greatest distances across the field. Sediment is the principal carrier of sorbed pesticides. The Universal Soil Loss Equation (USLE) developed by USDA is a simple method used to determine erosion losses. The USLE is most accurate for long-term average erosion losses.

The soil loss equation used in TFAT uses the modification described by Williams (1975). The Williams modification replaces the R (rainfall erosivity) term with an energy term. The energy term enables the estimation of event totals for erosion from the field. The modified universal soil loss equation (MUSLE) requires the remaining four USLE factors with no modifications.

TR--storm duration--This parameter is no longer required.

USLEK--soil erodibility factor--USLEK is a soil specific parameter. Specific values for various soils are obtainable from local Soil Conservation Service (SCS) offices. Approximate values (based on broad ranges of soil properties) can be estimated from Table 6-7.

USLELS--slope length and steepness factor--USLELS is a topographic parameter and is dimensionless. Values for LS can be estimated from Table 6-8.

USLEP--supporting practice factor--USLEP is a conservation supporting practice parameter and is dimensionless. Values range from 0.10 (extensive practices) to 1.0 (no supporting practice). Specific values for P can be estimated from Table 6-9.

USLEC--cover and management factor--USLEC is a management parameter and is dimensionless. Values range from 0.001 (well managed) to 1.0 (fallow or tilled condition). One value for each of the three growing periods (fallow,

TABLE 6-7. INDICATIONS OF THE GENERAL MAGNITUDE OF THE SOIL/ERODIBILITY FACTOR, K[a]

Texture Class	Organic Matter Content		
	<0.5%	2%	4%
	K	K	K
Sand	0.05	0.03	0.02
Fine Sand	.16	.14	.10
Very fine sand	.42	.36	.28
Loamy sand	.12	.10	.08
Loamy fine sand	.24	.20	.16
Loamy very fine sand	.44	.38	.30
Sandy loam	.27	.24	.19
Fine sandy loam	.35	.30	.24
Very fine sandy loam	.47	.41	.33
Loam	.38	.34	.29
Silt loam	.48	.42	.33
Silt	.60	.52	.42
Sandy clay loam	.27	.25	.21
Clay loam	.28	.25	.21
Silty clay loam	.37	.32	.26
Sandy clay	.14	.13	.12
Silty clay	.25	.23	.19
Clay		0.13-0.29	

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[a] The values shown are estimated averages of broad ranges of specific-soil values. When a texture is near the borderline of two texture classes, use the average of the two K values. For specific soils, Soil Conservation Service K-value tables will provide much greater accuracy. (Control of Water Pollution from Cropland, Vol. I, A Manual for Guideline Development. U.S. Environmental Protection Agency, Athens, GA. EPA-600/2-75-026a.)

cropping, residue) are required. Specific local values can be computed from Carsel et al. (1984) or obtained from the local SCS office. Generalized values are provided in Table 6-10.

CINTCP--maximum crop interception--The crop interception parameter (CINTCP) estimates the amount of rainfall that is intercepted by a fully developed plant canopy and retained on the plant surface, cms. A range of 0.1 - 0.3 cm for a dense crop canopy is reported USDA (1980). Values for several major crops are provided in Table 6-11.

TABLE 6-8. VALUES OF THE EROSION EQUATION'S TOPOGRAPHIC FACTOR, LS, FOR SPECIFIED COMBINATIONS OF SLOPE LENGTH AND STEEPNESS[a]

	Slope Length (feet)											
% Slope	25	50	75	100	150	200	300	400	500	600	800	1000
0.5	0.07	0.08	0.09	0.10	0.11	0.12	0.14	0.15	0.16	0.17	0.19	0.20
1	0.09	0.10	0.12	0.13	0.15	0.16	0.18	0.20	0.21	0.22	0.24	0.26
2	0.13	0.16	0.19	0.20	0.23	0.25	0.28	0.30	0.33	0.34	0.38	0.40
3	0.19	0.23	0.26	0.29	0.33	0.35	0.40	0.44	0.47	0.49	0.54	0.57
4	0.23	0.30	0.36	0.40	0.47	0.53	0.62	0.70	0.76	0.82	0.92	1.0
5	0.27	0.38	0.46	0.54	0.66	0.76	0.93	1.1	1.2	1.3	1.4	1.7
6	0.34	0.48	0.58	0.67	0.82	0.95	1.2	1.4	1.5	1.7	1.9	2.1
8	0.50	0.70	0.86	0.99	1.2	1.4	1.7	2.0	2.2	2.4	2.8	3.1
10	0.69	0.97	1.2	1.4	1.7	1.9	2.4	2.7	3.1	3.4	3.9	4.3
12	0.90	1.3	1.6	1.8	2.2	2.6	3.1	3.6	4.0	4.4	5.1	5.7
14	1.2	1.6	2.0	2.3	2.8	3.3	4.0	4.6	5.1	5.6	6.5	7.3
16	1.4	2.0	2.5	2.8	3.5	4.0	4.9	5.7	6.4	7.0	8.0	9.0
18	1.7	2.4	3.0	3.4	4.2	4.9	6.0	6.9	7.7	8.4	9.7	11.0
20	2.0	2.9	3.5	4.1	5.0	5.8	7.0	8.2	9.1	10.0	12.0	13.0
25	3.0	4.2	5.1	5.9	7.2	8.3	10.0	12.0	13.0	14.0	17.0	19.0
30	4.0	5.6	6.9	8.0	9.7	11.0	14.0	16.0	18.0	20.0	23.0	25.0
40	6.3	9.0	11.0	13.0	16.0	18.0	22.0	25.0	28.0	31.0	--	--
50	8.9	13.0	15.0	18.0	22.0	25.0	31.0	--	--	--	--	--
60	12.0	16.0	20.0	23.0	28.0	--	--	--	--	--	--	--

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[a] Values given for slopes longer than 300 feet or steeper than 18% are extrapolations beyond the range of the research data and, therefore, less certain than the others. (Control of Water Pollution from Cropland, Vol. I, A Manual for Guideline Development. U.S. Environmental Protection Agency, Athens, GA. EPA-600/275-026a.)

AMXDR--active crop rooting depth--PRZM requires input of the maximum active crop rooting depth (AMXDR), in centimeters, for the simulated crop (or the deepest root zone of multiple crop simulations) measured from the land surface. Generalized information for corn, soybeans, wheat, tobacco, grain sorghum, potatoes, peanuts, and cotton are provided in Table 6-12. If minor crops, such as mint, are simulated, or site specific information alters the generalized information, consulting with Carsel et al. (1984) or the Cooperative Extension Service in the specific locale is advisable.

TABLE 6-9. VALUES OF SUPPORT-PRACTICE FACTOR, P[a]

Practice	Land Slope (percent)				
	1.1-2	2.1-7	7.1-2	12.1-18	18.1-24
	(Factor P)				
Contouring (P_c)	0.60	0.50	0.60	0.80	0.90
Contour Strip cropping (P_{sc})[b]					
R-R-M-M$_1$	0.30	0.25	0.30	0.40	0.45
R-W-M-M	0.30	0.25	0.30	0.40	0.45
R-R-W-M	0.45	0.38	0.45	0.60	0.68
R-W	0.52	0.44	0.52	0.70	0.90
R-O	0.60	0.50	0.60	0.80	0.90
Contour listing or ridge planting (P_{cl})	0.30	0.25	0.30	0.40	0.45
Contour terracing (P_t)[c]	[d]$0.6/\sqrt{n}$	$0.5/\sqrt{n}$	$0.6/\sqrt{n}$	$0.8/\sqrt{n}$	$0.9/\sqrt{n}$
No support practice	1.0	1.0	1.0	1.0	1.0

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[a] Control of Water Pollution From Cropland, Vol. I, A Manual for Guideline Development. U.S. Environmental Protection Agency, Athens, GA. EPA-600/2-75-026a.

[b] R = rowcrop, W = fall-seeded grain, O = spring-seeded grain, M = meadow. The crops are grown in rotation and so arranged on the field that rowcrop strips are always separated by a meadow or winter-grain strip.

[c] These P_t values estimate the amount of soil eroded to the terrace channels and are used for conservation planning. For prediction of off-field sediment, the P_t values are multiplied by 0.2.

[d] n - number of approximately equal-length intervals into which the field slope is divided by the terraces. Tillage operations must be parallel to the terraces.

TABLE 6-10. GENERALIZED VALUES OF THE COVER AND MANAGEMENT FACTOR, C, IN THE 37 STATES EAST OF THE ROCKY MOUNTAINS[a,b]

Line No.	Crop, Rotation, and Management[c]	Productivity Level[d]	
		High	Mod.
		C value	
	Base value: continuous fallow, tilled up and down slope	1.00	1.00
	Corn		
1	C, RdR, fall TP, conv (1)	0.54	0.62
2	C, RdR, spring TP, conv (1)	.50	.59
3	C, RdL, fall TP, conv (1)	.42	.52
4	C, RdR, wc seeding, spring TP, conv (1)	.40	.49
5	C, RdL, standing, spring TP, conv (1)	.38	.48
6	C, fall shred stalks, spring TP, conv (1)	.35	.44
7	C(silage)-W(RdL, fall TP) (2)	.31	.35
8	C, RdL, fall chisel, spring disk, 40-30% rc (1)	.24	.30
9	C(silage), W wc seeding, no-till pl in c-k W (1)	.20	.24
10	C(RdL)-W)RdL, spring TP) (2)	.20	.28
11	C, fall shred stalks, chisel pl, 40-30% rc (1)	.19	.26
12	C-C-C-W-M, RdL, Tp for C, disk for W (5)	.17	.23
13	C, RdL, strip till row zones, 55-40% rc (1)	.16	.24
14	C-C-C-W-M-M, RdL, TP for C, disk for W (6)	.14	.20
15	C-C-W-M, RdL, TP for C, disk for W (4)	.12	.17
16	C, fall shred, no-till pl, 70-50% rc (1)	.11	.18
17	C-C-W-M-M, RdL, TP for C, disk for W (5)	.087	.14
18	C-C-C-W-M, RdL, no-till pl 2d & 3rd C (5)	.076	.13
19	C-C-W-M, RdL, no-till pl 2d C (4)	.068	.11
20	C, no-till pl in c-k wheat, 90-70% rc (1)	.062	.14
21	C-C-C-W-M-M, no-till pl 2d & 3rd C (6)	.061	.11
22	C-W-M, RdL, TP for C, disk for W (3)	.055	.095
23	C-C-W-M-M, RdL, no-till pl 2d C (5)	.051	.094
24	C-W-M-M, RdL, TP for C, disk for W (4)	.039	.074
25	C-W-M-M-M, RdL, TP for C, disk for W (5)	.032	.061
26	C, no-till pl in c-k sod, 95-80% rc (1)	.017	.053
	Cotton[e]		
27	Cot, conv (Western Plains) (1)	0.42	0.49
28	Cot, conv (South) (1)	.34	.40
	Meadow		
29	Grass & Legume mix	0.004	0.01
30	Alfalfa, lespedeza or Sericia	.020	
31	Sweet clover	.025	

TABLE 6-10. GENERALIZED VALUES OF THE COVER AND MANAGEMENT FACTOR, C, IN THE 37 STATES EAST OF THE ROCKY MOUNTAINS[a,b] (continued)

Line No.	Crop, Rotation, and Management[c]	Productivity Level[d] High	Productivity Level[d] Mod.
		C value	
Base value:	continuous fallow, tilled up and down slope	1.00	1.00
	Sorghum, grain (Western Plains)[e]		
32	RdL, spring TP, conv (1)	0.43	0.53
33	No-till pl in shredded 70-50%rc	.11	.18
	Soybeans[e]		
34	B, RdL, spring TP, conv (1)	0.48	0.54
35	C-B, TP annually, conv (2)	.43	.51
36	B, no-till pl	.22	.28
37	C-B, no-till pl, fall shred C stalks (2)	.18	.22
	Wheat		
38	W-F, fall TP after W (2)	0.38	
39	W-F, stubble mulch, 500 lbs rc (2)	.32	
40	W-F, stubble mulch, 1000 lbs rc (2)	.21	
41	Spring W, RdL, Sept TP, conv (N&S Dak) (1)	.23	
42	Winter W, RdL, Aug TP, conv (Kansas) (1)	.19	
43	Spring W, stubble mulch, 750 lbs rc (1)	.15	
44	Spring W, stubble mulch, 1250 lbs rc (1)	.12	
45	Winter W, stubble mulch, 750 lbs rc (1)	.11	
46	Winter W, stubble mulch, 1250 lbs rc (1)	.10	
47	W-M, conv (2)	.054	
48	W-M-M, conv (3)	.026	
49	W-M-M-M, conv (4)	.021	

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[a] This table is for illustrative purposes only and is not a complete list of cropping systems or potential practices. Values of C differ with rainfall pattern and planting dates. These generalized values show approximately the relative erosion-reducing effectiveness of various crop systems, but locationally derived C values should be used for conservation planning at the field level. Tables of local values are available from the Soil Conservation Service.

[b] Control of Water Pollution from Cropland, Vol. I, A Manual for Guideline Development. U.S. Environmental Protection Agency, Athens, GA. EPA-600/3-75-026a.

[c] Numbers in parentheses indicate number of years in the rotation cycle. No. (1) designates a continous one-crop system.

TABLE 6-10. GENERALIZED VALUES OF THE COVER AND MANAGEMENT FACTOR, C, IN THE 37 STATES EAST OF THE ROCKY MOUNTAINS[a,b] (concluded)

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[d] High level is exemplified by long-term yield averages greater than 75 bu. corn or 3 tons grass-and-legume hay; or cotton management that regularly provides good stands and growth.

[e] Grain sorghum, soybeans, or cotton may be substituted for corn in lines 12, 14, 15, 17-19, 21-25 to estimate C values for sod-based rotations.

Abbreviations defined:

B - soybeans

C - corn

c-k - chemically killed

conv - conventional

cot - cotton

F - fallow

M - grass & legume hay

pl - plant

W - wheat

we - winter cover

lbs rc - pounds of crop residue per acre remaining on surface after new crop seeding

% rc - percentage of soil surface covered by residue mulch after new crop seeding

70-50% rc - 70% cover for C values in first column; 50% for second column

RdR - residues (corn stover, straw, etc.) removed or burned

RdL - all residues left on field (on surface or incorporated)

TP - turn plowed (upper 5 or more inches of soil inverted, covering residues)

TABLE 6-11. INTERCEPTION STORAGE FOR MAJOR CROPS

Crop	Density	CINTCP (cm)
Corn	Heavy	0.25 - 0.30
Soybeans	Moderate	0.20 - 0.25
Wheat	Light	0.0 - 0.15
Oats	Light	0.0 - 0.15
Barley	Light	0.0 - 0.15
Potatoes	Light	0.0 - 0.15
Peanuts	Light	0.0 - 0.15
Cotton	Moderate	0.20 - 0.25
Tobacco	Moderate	0.20 - 0.25

CN--runoff curve number--The interaction of hydrologic soil group (soil) and land use and treatment (cover) is accounted for by assigning a runoff curve number (CN) for average soil moisture condition (AMC II) to important soil cover complexes for the fallow, cropping, and residue parts of a growing season. The average curve numbers for each of the three soil cover complexes are estimated using Tables 6-13 through 6-17. The following steps provide a procedure for obtaining the correct curve numbers. Corn planted in straight rows will be used as an example.

Step 1. From Appendix B (Carsel et al. 1984) find the hydrologic soil group for the particular soil that is in the area under consideration (Appendix B from this reference contains a listing of soil groups and their hydrologic soil cover classification). There are four different soil classifications (A, B, C, D) and are in the order of decreasing percolation potential and increasing slope and runoff potential. Soil characteristics associated with each hydrologic group are as follows.

Group A: Deep sand, deep loess, aggregated silts, minimum infiltration of 0.76 - 1.14 (cm hr^{-1})

TABLE 6-12. AGRONOMIC DATA FOR MAJOR AGRICULTURAL CROPS IN THE UNITED STATES

Crop	Representative States of Major States Production[a]	Planting Window, Month, Day (Julian Day)[b]	Crop Emergence (Days from Planting)	Crop Maturity (Days from Planting)	Harvest Window, Month, Day (Julian Day)[b]	Average Yield/Acre 1977-1979[c]	Range of Active Plant Rooting Depth (cm)
Corn	IA, IL, IN NE, OH	April 25 (115) to June 15 (166)	5-15	110-130	Sept. 25 (268 to Dec. 10 (344)	110 bu	60-120
Soybeans	IA, IL, IN, MS, OH	May 1 (121) to June 25 (176)	5-15	110-130	Sept. 15 (258) to Dec. 10 (344)	35 bu	30-60
Cotton	TX, MS, CA, AZ, AR	March 1 (60) to May 25 (145) [TX to June 20 (171)]	5-15	110-130	Sept. 1 (244) to Jan. 15 (015) [TX Aug. 1 (213) to Dec. 20 (354)]	670 lbs	30-90
Wheat	KS, OK, CA, ND, MT, WA, MN, ID	Aug. 15 (227) to Oct. 25 (298) [WA to Nov. 20 (324), CA to Feb. 15 (046]	5-15	200-225	June 15 (166) to Sept. 20 (263)	40 bu	15-30
Potatoes	Long Island NY, ME, ID, WA, CA, OR	April 1 (091) to May 1 (121)	5-15	150-170	Sept. 1 (244) to Oct. 1 (274)	335 cwt	15-45
Peanuts	GA, TX, AL, NC, VA	April 5 (095) to June 5 (156) [TX Mar. 31 (090) to July 20 (201)]	5-15	150-175	Aug. 10 (222) to Dec. 15 (349)	2550 lbs	30-60
Tobacco	NC, SC, TN, KY, VA	April 5 (095) to June 20 (171)	Planted in Field as Seedling	120-150	July 1 (182) to Oct. 1 (274)	2000 lbs	30-60
Grain Sorghum	TX, KS, NE	TX Mar. 1 (060) to July 1 (182) KS, NE May 5 (125) to July 1 (182)	5-15	120-150	TX July 1 (182) to Nov. 20 (324) KS, NE Sept. 20 (263) to Dec. 1 (335)	62 bu	15-30

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[a] Bay, D.M. and Bellinghausen, R.P. Missouri Farm Facts. Missouri Department of Agriculture. May 1979.

[b] Burkhead, B.E., Max, R.C., Karnes, R.B., and Neid, E. Usual Planting and Harvesting Dates. USDA, Agricultural Handbook No. 283. 1972.

[c] Kirkbride, J.W. (Ed.). Crop Production Annual Summary. USDA, Crop Reporting Board Publication CrPr 2-1. 1980.

TABLE 6-13. RUNOFF CURVE NUMBERS FOR HYDROLOGIC SOIL-COVER COMPLEXES[a] (ANTECEDENT MOISTURE CONDITION II, AND $I_a = 0.2$ S)

Cover			Hydrologic Soil Group			
Land Use	Treatment or Practice	Hydrologic Condition	A	B	C	D
Fallow	Straight Row	---	77	86	91	94
Row crops	Straight Row	Poor	72	78	85	91
	Straight row	Good	67	78	85	89
	Contoured	Poor	70	79	84	88
	Contoured	Good	65	75	82	86
	Contoured and terraced	Poor	66	74	80	82
	Contoured and terraced	Good	62	71	78	81
Small grain	Straight row	Poor	65	76	84	88
	Straight row	Good	63	75	83	87
	Contoured	Poor	63	74	83	87
	Contoured	Good	61	73	81	84
	Contoured and terraced	Poor	61	72	79	82
	Contoured and terraced	Good	59	70	78	81
Close-seeded legumes[b] or rotation meadow	Straight row	Poor	66	77	85	89
	Straight row	Good	58	72	81	85
	Contoured	Poor	64	75	83	85
	Contoured	Good	55	69	78	83
	Contoured and terraced	Poor	63	73	80	83
	Contoured and terraced	Good	51	67	76	80
Pasture or range		Poor	68	79	86	89
		Fair	49	69	79	84
		Good	39	61	74	80
	Contoured	Poor	47	67	81	88
	Contoured	Fair	25	59	75	83
	Contoured	Good	6	35	70	79
Meadow		Good	30	58	71	78
Woods		Poor	45	66	77	83
		Fair	36	60	73	79
		Good	25	55	70	77
Farmsteads		----	59	74	82	86
Roads (dirt)[c]		----	72	82	87	89
(hard surface)[c]		----	74	84	90	92

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[a] Soil Conservation Service, USDA. SCS National Engineering Handbook, Handbook, Section 4, Hydrology. 1972.

[b] Close-drilled or broadcast.

[c] Including right-of-way.

TABLE 6-14. METHOD FOR CONVERTING CROP YIELDS TO RESIDUE[a]

Crop[b]	Straw/Grain Ratio	Bushel Weight (lbs)
Barley	1.5	48
Corn	1.0	56
Oats	2.0	32
Rice	1.5	45
Rye	1.5	56
Sorghum	1.0	56
Soybeans	1.5	60
Winter wheat	1.7	60
Spring Wheat	1.3	60

[a] Crop residue = (straw/grain ratio) x (bushel weight in lb/bu) x (crop yield in bu/acre).

[b] Knisel, W.G. (Ed.). CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. USDA, Conservation Research Report No. 26, 1980.

TABLE 6-15. RESIDUE REMAINING FROM TILLAGE OPERATIONS[a]

Tillage[b] Operation	Residue Remaining (%)
Chisel Plow	65
Rod weeder	90
Light disk	70
Heavy disk	30
Moldboard plow	10
Till plant	80
Fluted coulter	90
V Sweep	90

[a] Crop residue remaining = (crop residue from Table 10) x (tillage factor(s).

[b] Knisel, W.G. (Ed.). CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. USDA, Conservation Research Report No. 26, 1980.

Group B: Shallow loess, sandy loam, minimum infiltration 0.38 - 0.76 (cm hr^{-1}).

Group C: Clay loams, shallow sandy loam, soils low in organic content, and soils usually high in clay, minimum infiltration 0.13 - 0.38 (cm hr^{-1}).

Group D: Soils that swell significantly when wet, heavy plastic clays, and certain saline soils, minimum infiltration 0.03 - 0.13 (cm hr^{-1}).

If the soil series or soil properties are not known, the hydrologic soil group can be estimated from Figure 6.3.

Table 6-16. REDUCTION IN RUNOFF CURVE NUMBERS CAUSED BY CONSERVATION TILLAGE AND RESIDUE MANAGEMENT[a]

Large Residue Crop[b] (lb/acre)	Medium Residue Crop[c] (lb/acre)	Surface Covered by Residue (%)	Reduction in Curve Number[d] (%)
0	0	0	0
400	150	10	0
700	300	19	2
1,100	450	28	4
1,500	700	37	6
2,000	950	46	8
2,500	1,200	55	10
6,200	3,500	90	10

[a] Knisel, W.G. (Ed.). CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. USDA, Conservation Research Report No. 26, 1980.

[b] Large-residue crop (corn).

[c] Medium residue crop (wheat, oats, barley, rye, sorghum, soybeans).

[d] Percent reduction in curve numbers can be interpolated linearly. Only apply 0 to 1/2 of these percent reductions to CNs for contouring and terracing practices when they are used in conjunction with conservation tillage.

TABLE 6-17. VALUES FOR ESTIMATING WFMAX IN EXPONENTIAL FOLIAR MODEL

Crop	Yield[a] (Bu/Ac)	Bushel[a] dry wt. (lbs/Bu)	Straw/Grain Ratio	Units Conversion Factor	WFMAX
Corn	110	56	1.0	1.1214×10^{-4}	1.38
Sorghum	62	56	1.0	1.1214×10^{-4}	0.78
Soybeans	35	60	1.5	1.1214×10^{-4}	0.59
Winter wheat	40	60	1.7	1.1214×10^{-4}	0.72

[a] 10-year average

Care must be exercised, however in use of this figure. Considerable spatial aggregation was made in order to develop the generalized map over such a large area. Where possible, development of more highly resolved data is preferable.

Step 2. From Table 6-13 find the land use and treatment or practice that is to be simulated (e.g., row crops, straight row).

Step 3. From Table 6-13 find the hydrologic condition of the soil that is to be simulated (e.g., good).

Step 4. From Table 6-13 find the curve number for antecedent moisture condition II for the site selected. Example: Hydrologic group = A, treatment practice is straight row, land use is row crops, hydrologic condition is good. The curve number for the cropping season is 67.

Step 5. Follow the same procedure for the fallow portion of the growing season using only the hydrologic soil group. Example: Hydrologic soil group A, land use fallow, curve number for condition II is 77.

Step 6. The post-harvest or residue portions of the year requires numbers that reflect the extent of surface cover after harvest. This can be quite variable and in many, cases may

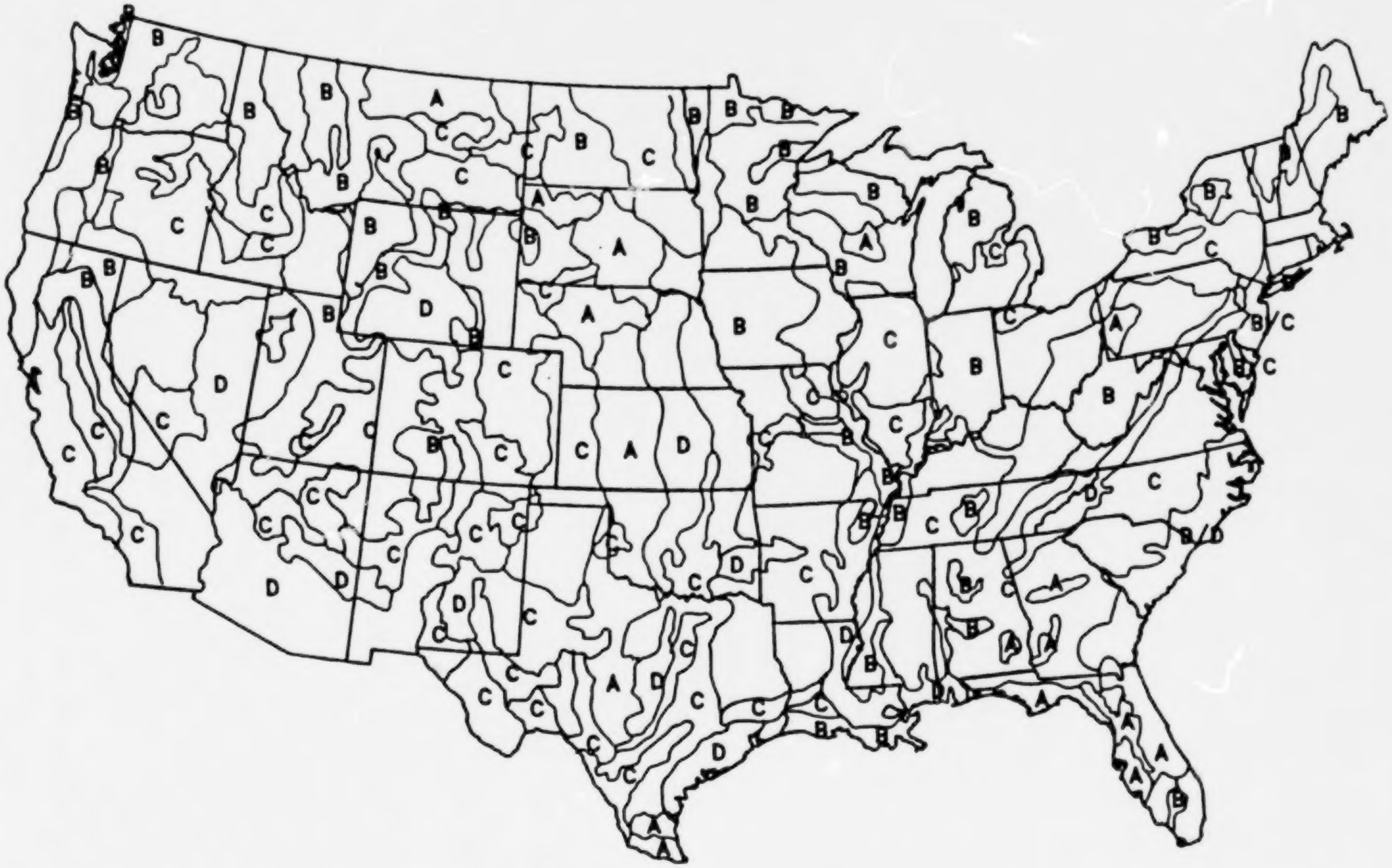

Figure 6.3 Diagram for estimating Soil Conservation Service soil hydrologic groups. (From EPA Field Guide for Scientific Support Activities Associated with Superfund Emergency Response. U.S. Environmental Protection Agency, Corvallis OR, EPA-600/8-82-025.)

require considerable judgement. Under "average" conditions a value set to the mean of the fallow and growing period numbers (from steps 4, 5) is appropriate. In the example case, this number will be the mean of 77 and 67, or 72.

Step 7. The curve number input sequence is now written as

77 67 72

Additional guidance for management practices

Pesticides are being increasingly used in conjunction with conservation practices to reduce erosion and runoff. Most notable among these practices is the use of conservation tillage. The idea is to increase the soil surface residue and hence reduce erosion and runoff by increasing infiltration. The curve numbers developed in steps 1-7 assume conventional practices and must be further modified to reflect the changes in management. Both the fall and growing season numbers must be modified. For purposes of this example, assume the corn is produced by using chisel plows rather than the conventional tillage assumed above. The following steps now apply.

Step 8. From Table 6-14 find the straw/grain ratio for corn, which is 1.0.

Step 9. From Table 6-14 find the bushel weight of corn, which is 56.

Step 10. From Table 6-12 find bushel/acre yield of corn, which is 110.

Step 11. Multiply straw/grain ratio * bushel weight *" bushel weight/acre = crop residue produced by the crop. For corn, 1.0 x 56 x 110 = 6160.

Step 12. From Table 6-15 find the tillage practice desired for the crop use site (e.g. chisel plow).

Step 13. Multiply the crop residue determined in step 11 by the tillage factor from step 12 to determine residue remaining, i.e, 6160 x 0.65 = 4004.

Step 14. From Table 6-16 find the reduction in curve number for AMC II, crop curve number produced from residue remaining after harvest determined in step 12. For corn at 4000 pounds per acre, a 10% reduction in curve number is produced.

Step 15. Determine the curve number for antecedent moisture condition (AMC) II. From Steps 1 - 5, AMC II was 67. 67 * 0.10 = 6.7, which is rounded to 7.0. The modified curve numbers are 67 - 7 = 60 and 77 - 7 = 70.

Step 16. The post-harvest curve number must also now be reduced by averaging the fallow and growing season numbers, that is, 70 and 60 to yield 65.

COVMAX--maximum areal crop coverage--TFAT estimates the ground cover as the crop grows to some maximum value, COVMAX, by calling the PLTGRN routine. COVMAX is passed through TFAT to this module. The maximum areal coverage (COVMAX) determines the fraction of ground covered by the crop and thus influences the mass of pesticide that reaches the ground from an application event. For most crops, the maximum coverage will be on the order of 80 to 100 percent.

WFMAX--maximum foliar dry weight--If the user chooses to have the model estimate the distribution between plants and the soil by an exponential function, then WFMAX must be specified. WFMAX must be entered here whether PLTGLN or the original PRZM plant growth model is used.

The maximum foliar dry weight, WFMAX, of the plant above ground (kg m^{-2}) is the exponent used in the exponential foliar pesticide application model. WFMAX for several major crops is given in Table 6-17. Estimates for other crops will require yield information that is available from from USDA crop reporting service. WFMAX is computed by finding the product of columns 2, 3, and 5, and by multiplying this number by the straw/grain ratio (col. 4) plus 1.0. The straw/grain ratio defines the amount of straw associated with the final grain product. Both the straw and grain should be accounted for to determine the maximum weight. Thus, the straw-to-grain ratio should have (1.0) added to it when used to compute WFMAX. An example is provided for barley.

Step 1. Yield, bushel dry wt., and straw/grain ratio for barley are 42.0, 48.0, and 1.5, respectively.

Step 2. WFMAX = Bu/Ac * Lbs/Bu * (straw/grain ratio + 1.) * conversion factor to yield (kg m^{-2}) for TFAT input.

Step 3. Conversion factor $= 2.47\ \frac{Ac}{ha} * \frac{1\ ha}{10^4 m^2} * \frac{0.454\ kg}{Lbs} =$

$$1.1214 \times 10^{-4}.$$

Step 4. WFMAX $= 42.0 * 48.0 * (1.5 + 1.0) * 1.1214 \times 10^{-4}$, which equals 0.56.

EMD, EMM, IYREM, MAD, MAM, IYRMAT, HAD, HAM, IYRHAR--cropping information for emergence, maturity, and harvest--Generalized cropping information including date of emergence (EMD, EMM, IYREM), maturity (MAD, MAM, IYRMAT), and harvest (HAD, HAM, IYRHAR) for eight major crops including corn, soybeans, wheat, tobacco, grain sorghum, potatoes, and peanuts are provided in Table 6-12. Simulations involving minor crops such as mint, or where site specific information alters the general practices provided, may require consultation with Carsel et al. (1984) or the local Cooperative Extension Service. The user should note that if the PLTGRN option is on, the crop maturation information is not utilized.

6.4.1.3 Pesticide Parameters--

Pesticides can be applied directly to the soil surface, the plant canopy, or to both. Two modeling problems arise when one considers this. First, the initial distribution of the applied pesticide between plant foliage and the soil surface must be estimated. Second, the remaining foliar deposited pesticides then become available for degradation (photolysis) or removal (volatilization, washoff). Recall that two options are available for distributing the applied pesticide (the FAM parameter).

TAPP--total pesticide application--The total pesticide application per event is entered in terms of kg-active ingredient (a.i.) ha^{-1}. Typical application rates are included on the product's registration label. According to Smith (1988, personal communication) the coefficient of variation for granular application is 40 to 70% for spray application.

DEPI--depth of incorporation--This variable is only needed if soil application of chemical is specified (i.e., FAM = 1). Typical incorporation depths are 5-10 cm. If soil injection is being simulated, user should be aware that injection below 15 to 20 cm is difficult to achieve and represents an approximate upper limit of incorporation depth (Matthews 1979). Representative values for several soil application methods are given in Table 6-18.

BETA--canopy penetration attenuation constant--The attenuation coefficient, β, depends mainly upon the leaf area index (LAI)--the higher the LAI, the higher will be the value of β. Uk and Courshee (1982) report

TABLE 6-18. PESTICIDE SOIL APPLICATION METHODS AND DISTRIBUTION

Method of Application	Common Procedure	Distribution	DEPI
Broadcast	Spread as dry granules or spray over the whole surface	Remains on the soil surface	0.0
Disked-in	Disking after broadcast application	Assume uniform distribution to tillage depth (10 cm)	10.0
Chisel-plowed	Chisel plowing after broadcast	Assume linear distribution to tillage depth (15 cm)	15.0
Surface banded	Spread as dry granules or a spray over a fraction of the row	Remains on soil surface	0.0
Banded incorporated	Spread as dry granules or a spray over a fraction of the row and incorporated in planting operation	Assume uniform distribution to depth of incorporation (5 cm)	5.0

an attenuation coefficient of 0.018 cm^{-1} for a cotton crop having an LAI of 3 to 4 and 0.042 cm^{-1} for a cotton crop having an LAI of 6.

FILTRA--initial foliage to soil distribution--The filtration parameter (FILTRA) relates to the equation for partitioning the applied pesticide between the foliage and ground (this applies when FAM = 3). Lassey (1982) suggests values in the range of 2.3 - 3.3 $m^2\ kg^{-1}$. Most of the variation appears to be due to the vegetation and not the aerosol. The user should note that the value of FILTRA entered here only applies to pesticide application events specified in the TFAT habitat input sequence. If application events are specified from the GRDDEP module, then a corresponding value of this parameter would be entered there, given that the user wishes to invoke the exponential deposition model.

FEXTRC--foliar washoff extraction coefficient--Washoff from plant surfaces is modeled using a relationship among rainfall, foliar mass of pesticide, and an extraction coefficient. The parameter (FEXTRC) is the required input parameter to estimate the flux of pesticide washoff. Exact values are varied and depend upon the crop, pesticide properties, and application method. Smith and Carsel (1984) suggest 0.10 is suitable for most pesticides.

PLDKRT--foliar disappearance rate constant--The degradation of pesticides on plant surfaces is modeled by a simple first-order rate expression. This is a very chemical specific parameter that must be measured. Typical values for selected pesticides are provided in Table 6-19.

If the user has monitoring data which shows the degradation of plant foliar concentrations with time, then the coefficient can be calibrated to cause the simulated concentrations to mimic the observed data. The exponential decay model is given by:

$$C = C_o e^{-(FEXTRC)t} \qquad (6\text{-}6)$$

in which C is the simulated concentration
C_o is the initial concentration
FEXTRC is the first order decay rate (day^{-1}) and
t is the time elapsed since application (days)

In linear form the equation is

$$\ln\left({}^{C}/_{C_o}\right) = -(FEXTRC)t \qquad (6\text{-}7)$$

Therefore, the coefficient FEXTRC is the slope of the plot of the natural log of the normalized concentrations (C/C_o) vs. time in days.

KD--pesticide soil-water distribution coefficient--The user can enter directly the distribution coefficient or the model will calculate a value given other pesticide properties. If the parameter KDFLAG is set to a valu of 0, then direct data input is made as the parameter KD. If KDFLAG is set to 1, however, additional information is required.

PCMC, SOL--options for use in estimating distribution coefficients from related input data--The fate of pesticides in soil and water is highly dependent on the sorptive characteristics of the compound. Sorptive characteristics affect the physical movement of pesticides significantly. The sorptive properties of pesticides generally correlate well with the organic carbon content of soils. The carbon content of most soils decreases with depth.

The TFAT module allows the user to estimate an organic carbon partition coefficient for the pesticide from one of three models based on water solubility. The K_{oc} is subsequently multiplied by organic carbon to obtain the partition coefficient. The three models are:

PCMC1 $$\text{Log } K_{oc} = (-0.54 * \text{Log SOL}) + 0.44 \tag{6-8}$$

where K_{oc} = organic carbon distribution coefficient
SOL = water solubility, mole fraction

TABLE 6-19. DEGRADATION RATE CONSTANTS OF SELECTED PESTICIDES ON FOLIAGE[a]

Class	Group	Decay Rate (days^{-1})
Organochloride	Fast (aldrin, dieldrin, ethylan, heptachlor, lindane, methoxychlor).	0.231 - 0.1386
	Slow (chlordane, DDT, endrin, toxaphene).	0.1195 - 0.0510
Organophosphate	Fast (acepate, chlorphyrifos-methyl, cyanophenphos, diazinon, depterex, ethion, fenitrothion, leptophos, malathion, methidathion, methyl parathion, phorate, phosdrin, phosphamidon, quinalphos, alithion, tokuthion, triazophos, trithion).	0.2772 - 0.3013
	Slow (azinphosmethyl, demeton, dimethoate, EPN, phosalone).	0.1925 - 0.0541
Carbamate	Fast (carbofuran)	0.630
	Slow (carbaryl)	0.1260 - 0.0855
Pyrethroid	(permethrin)	0.0196
Pyridine	(pichloram)	0.0866
Benzoic acid	(dicamba)	0.0745

[a] Knisel, W.G. (Ed.). CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. USDA, Conservation Research Report No. 26, 1980.

PCMC2 $\text{Log } K_{oc} = 3.64 - (0.55 * \text{Log SOL})$ (6-9)

where SOL = water solubility, milligrams liter^{-1}

PCMC3 $\text{Log } K_{oc} = 4.40 - (0.557 * \text{Log SOL})$ (6-10)

where SOL = water solubility, micromoles liter^{-1}

These models are selected by setting PCMC to values of 1, 2, or 3, respectively. These methods were selected because of referenced documentation and provisions for direct use with the most commonly reported physical pesticide parameter, water solubility. The three models used in TFAT for estimating partitioning between soil and water are limited to specific types of pesticides. These equations are best used for pesticides having melting points below 120 °C. Solubilities above these temperatures are affected by crystalline energy and other such physical properties. The three models are not appropriate for pesticides whose solubilities are affected by crystalline energy or other physical properties, and would have a tendency to overestimate the partitioning between soil and water. Of the three models, the first model is for true equilibrium of completely dispersed particles of soil/water concentrations less than 10.0 g l^{-1}. The second and third models are for soil/water concentrations greater than 10.0 g l^{-1} and for short equilibrium periods of 48 hours or less. For most applications, the first model would be the most appropriate.

Some pesticides having properties amenable for use with the water solubility models are provided in Table 6-20. The pesticide solubility, SOL, must also be input. Units must be consistent with the model chosen. Table 6-20 also provides pertinent values for the selected pesticides.

The user should be aware that an organic carbon partition coefficient is also expected by the plant translocation model. The values selected for use in the two respective parts of the program should be consistent, unless the user has information to the contrary.

KD user-specified distribution coefficients--A useful relationship exists between the octanol-water distribution coefficient and the organic carbon distribution coefficient. This relationship can be used when measured soil distribution coefficients are not available, or the pesticides posses crystalline energy properties that would preclude the use of any water solubility models.

The octanol-water distribution coefficient can be used for calculating distribution coefficients for pesticides that possess monomer-associated properties for solubility in water. Karickhoff et al. (1979) proposed a relationship between K_{ow} and K_{oc} given by

TABLE 6-20. PHYSICAL CHARACTERISTICS OF SELECTED PESTICIDES FOR USE IN DEVELOPMENT OF PARTITION COEFFICIENTS (USING WATER SOLUBILITY) AND REPORTED DEGRADATION RATE CONSTANTS IN SOIL ROOT ZONE

Chemical	Common Name	Solubility in Water (Temp. 20-25°C) (mg/l)	Reference	Mode of Action: Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	Partitioning Model: PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (um/l)	Degradation Rate Constant in Soil Root Zone (days^{-1})	Reference
Actellic	pirimiphos-methyl	5	a	X					274	b	3.28×10^{-7}	5	18		
Alachlor	alachlor	220	b		X				269.9	b	1.47×10^{-5}	220	815	.0384	f
Antor	diethatyl ethyl	105	a		X				311.5	c	6.07×10^{-6}	105	337	.0099-.0173	g
Aresin	monolinuron	735	a		X				214.6	b	6.17×10^{-5}	735	3430		
Balan	benefin	70	b		X				335.3	b	3.76×10^{-6}	70	209	0.3349	f
Basalin	fluchloralin	0.7	b		X				355.7	b	3.55×10^{-8}	0.7	2	0.0169	f
Baygon	propoxur	2000	a	X					209	b	1.72×10^{-4}	2000	9600		
Baygon Meb	pilfenate	50	a	X					336.2	d	2.68×10^{-6}	50	149		
Bayleton	triadimefon	70	a			X			267.45	d	4.72×10^{-6}	70	262		
Baythion	phoxim	7	b	X					298	b	4.23×10^{-7}	7	24		
Baythion C	chlorphoxim	1.7	a	X					301.45	d	1.02×10^{-7}	1.7	5.6		
Betasan	bensulide	25	c		X				397.5	b	1.13×10^{-6}	25	63		
Bromophos	bromophos	40	a	X					366	b	1.97×10^{-6}	40	109	.0198	f
Butachlor	butachlor	23	a		X				312	e	1.33×10^{-6}	23	74		
Bux	bufencarb	1	b	X					221.3	b	8.14×10^{-8}	1.0	5		
Carbamult	promecarb	92	a	X					207	d	8.01×10^{-6}	92	444		
Carbyne	barban	11	c		X				258.1	b	7.70×10^{-7}	11	43	.0347	g
Chlordimeform	chlordimeform	250	a	X				X	196.7	b	2.30×10^{-5}	250	1270		
Chlorfenvinphos	chlorfenvinphos	110	a	X					359.5	b	5.51×10^{-6}	110	306	.0055	f
Chloro IPC	chlorpropham	108	b		X				213.7	b	9.11×10^{-6}	108	505	.0058-.00267	g
Chlorpyrifos	chlorpyrifos	2	b	X					350.5	b	1.03×10^{-7}	2.0	6		
Co-Ral	coumaphos	1.5	b	X					362.8	b	7.45×10^{-8}	1.5	4		
Counter	terbufos	15	a	X			X		288	d	9.38×10^{-7}	15	52		
DNOC	DNOC	130	a	X	X	X			198.1	b	1.18×10^{-5}	130	656		
Dichlorprop	dichlorprop	350	a		X				235	b	2.68×10^{-5}	350	1490	.0578-.0866	f
Dimetan	dimetan	30000	b	X					197.3	b	2.74×10^{-3}	30000	152000		
Dimethoate	dimethoate	X=25000	a	X					229.1	b	1.97×10^{-3}	25000	109000	.0057	
Dinitramine	dinitroamine	1	a		X				322.2	c	5.60×10^{-8}	1	3	.0193-.0856	f
Dinoseb	dinoseb	52	c		X				240.2	b	3.90×10^{-6}	52	217	.0462-.0231	g
Dazomet	dazomet	1200	b		X	X	X		162.3	b	1.33×10^{-4}	1200	7390		
Devrinol	napropamide	73	a		X				271.36		4.85×10^{-6}	73	269		
Elocron	dioxacarb	6000	a	X					223	b	4.85×10^{-4}	6000	26900	.3465-.0248	f
Evik	ametryn	185	a		X				227	b	1.47×10^{-5}	185	815	.0231-.0077	g

TABLE 6-20. PHYSICAL CHARACTERISTICS OF SELECTED PESTICIDES FOR USE IN DEVELOPMENT OF PARTITION COEFFICIENTS (USING WATER SOLUBILITY) AND REPORTED DEGRADATION RATE CONSTANTS IN SOIL ROOT ZONE

			Mode of Action								Partitioning Model				
Chemical	Common Name	Solubility in Water (Temp. 20-25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (um/l)	Degradation Rate Constant in Soil Root Zone (days^{-1})	Reference
Far-Go	triallate	4	b		X				304.6	b	2.37×10^{-7}	4	13	.0231-.0713	g
Fongarid	furalaxyl	230	a			X			301	d	1.38×10^{-5}	230	764		
Fornothion	fornothion	2600	a	X				X	257	b	1.82×10^{-4}	2600	10100		
Fuji-one	isoprothiolane	48	a	X		X			290	d	2.98×10^{-6}	48	166		
Gardona	tetrachlorvinphos	11	b	X					366	b	5.42×10^{-7}	11	30	.1732-.1386	
Gesaran	methoprotryne	320	a		X				271	b	2.13×10^{-5}	320	1180		
Goal	oxyfluorfen	0.1	c		X				361.7	c	4.98×10^{-9}	0.1	0.3	.0231-.0173	c
Guthion	azinphos-methyl	29	a	X					317.3	b	1.65×10^{-6}	29	91	.0533-.0014	f
Hoelon	diclofop methyl	30	a		X				340.9	d	1.59×10^{-6}	30	88		
Imidan	phosmet	25	b	X					317.3	b	1.42×10^{-6}	25	79		
IPC	propham	250	b		X				179.2	b	2.51×10^{-5}	250	1400	.0347-.0116	g
Linuron	linuron	75	a		X				249.1	b	5.42×10^{-6}	75	300	.0280-.0039	f
Malathion	malathion	145	a	X					330.4	b	7.91×10^{-6}	145	439	2.91-.4152	f
Mecoprop	mecoprop	620	a		X				214.6	b	5.21×10^{-5}	620	2890		
MEMC	MEMC	50000	a			X			295	d	3.05×10^{-3}	50000	169000		
Merpelan AZ	isocarbamid	13000	a		X				185	d	1.27×10^{-3}	13000	70300		
Mesoranil	aziprotryn	75	b		X				225	b	6.01×10^{-6}	75	333		
Mesurol	mercaptodimethur	2.7×10^{7}	a	X					225.3	b	2.16	2.7×10^{7}	1.2×10^{8}		
Methomyl	methomyl	58000	a	X					162.2	b	6.44×10^{-3}	58000	358000		
Methoxychlor	methoxychlor	0.1	b	X					345.7	b	5.21×10^{-9}	0.1	0.3	.0046-.0033	f
Meth-Parathion	methyl Parathion	$\bar{X} = 57.5$	a	X					263.2	b	3.94×10^{-6}	57.5	219	.2207	f
Nemacur	fenamiphos	400	a			X			303	b	2.38×10^{-5}	400	1320		
Nortron	ethofumesate	110	a		X				286	d	6.93×10^{-6}	110	385		
Orthene	acephate	6.5×10^{5}	b	X					183.2	b	0.06	6.5×10^{5}	3550000		
Oxamyl	oxamyl	2.8×10^{5}	a	X			X	X	219	b	0.023	2.8×10^{5}	1280000	.0354-.0646	f
Parathion	parathion	24	b	X					291.3	b	1.48×10^{-6}	24	82	.2962-.0046	f
Patoran	metabromuron	330	a		X				258.9	d	2.30×10^{-5}	330	1280	.0234	f
Phorate	phorate	50	b	X					260.4	b	3.46×10^{-6}	50	192	.0363-.0040	f
Propachlor	propachlor	580	c		X				211.7	b	4.94×10^{-5}	580	2740	.0231-.0139	g
Propanil	propanil	500	c		X				218	b	4.13×10^{-5}	500	2290	.693-.231	g
Prowl	pendimethalin	0.5	c		X				281.3	c	3.20×10^{-8}	0.5	1.8		
Prynachlor	prynachlor	500	a		X				221.7	b	4.06×10^{-5}	500	2260		

TABLE 6-20. PHYSICAL CHARACTERISTICS OF SELECTED PESTICIDES FOR USE IN DEVELOPMENT OF PARTITION COEFFICIENTS (USING WATER SOLUBILITY) AND REPORTED DEGRADATION RATE CONSTANTS IN SOIL ROOT ZONE

Chemical	Common Name	Solubility in Water (Temp. 20-25°C) (mg/l)	Mode of Action: Reference	Mode of Action: Insecticide	Mode of Action: Herbicide	Mode of Action: Fungicide	Mode of Action: Nematocide	Mode of Action: Acaricide	Molecular weight (g)	Reference	Partitioning Model: PCMC1 (mole fraction)	Partitioning Model: PMCM2 (mg/l)	Partitioning Model: PCMC3 (um/l)	Degradation Rate Constant in Soil Root Zone (days^{-1})	Reference
Quinalphos	quinalphos	22	a	X				X	298	d	1.33×10^{-6}	22	74		
Ronstar	oxadiazon	0.7	b		X				345.23	b	3.65×10^{-8}	0.7	2.0		
Sancap	dipropetryn	16	a		X				255.4	b	1.13×10^{-6}	16	63		
Semeron	desmetryn	580	a		X				213	b	4.91×10^{-5}	580	2720		
Supracide	methidathion	240	a	X				X	302	b	1.43×10^{-5}	240	795	.0495-.0108	f
Tachigareu	hymexazol	85000	a			X			99.05	b	0.02	85000	858000		
Temik	aldicarb	6000	a	X			X	X	190.3	b	5.68×10^{-4}	6000	31500	.0322-.0116	f
Tolban	profluralin	0.1	a		X				347.3	c	5.19×10^{-9}	0.1	0.3	.0049	f
Trifluralin	trifluralin	24	b		X				335.3	b	1.29×10^{-6}	24	71	.0956-.0026	f
Tsumacide	MTMC	2600	a	X					165	d	2.84×10^{-4}	2600	15800		
Tordon	picloram	430	c		X				241.5	b	3.21×10^{-5}	430	1780	.0354-.0019	f
Toxaphene	toxaphene	3	b	X					413	b	1.31×10^{-7}	3	7	.0046	f
Trichlorfon	trichlorfon	120000	a	X					257.35	d	8.40×10^{-3}	120000	466000		

Calculations for the Karickhoff and Chiou partitioning equations are:

PCMC1: $\frac{\text{ppm solubility}}{\text{molecular weight (g)}}$ = millimole solubility (MMS)

$\frac{\text{MMS}}{10^3}$ = molar solubility (MS) $\frac{\text{MS}}{\text{55.5 (molar conc. water)}}$ = mole fraction

Chiou: $\frac{\text{ppm solubility}}{\text{molecular weight (g)}}$ = millimole solubility (MMS)

$\frac{\text{MMS}}{10^3} \times 10^6$ = um/l

References

[a] Farm Chemical Handbook, Meister Publishing Company, Willoughby, OH (1981).

[b] Pesticide Manual, Issued by the British Crop Protection Council, 1968.

TABLE 6-20. PHYSICAL CHARACTERISTICS OF SELECTED PESTICIDES FOR USE IN DEVELOPMENT OF PARTITION COEFFICIENTS (USING WATER SOLUBILITY) AND REPORTED DEGRADATION RATE CONSTANTS IN SOIL ROOT ZONE

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[c] Herbicide Handbook of the Weed Science Society of America, 4th ed. 1979.

[d] Calculations based on information from Farm Chemical Handbook, 1981.

[e] Analytical Reference Standards and Supplemental Data for Pesticides and Other Organic Compounds, U.S. EPA-600/2-81-011, 1981.

[f] Nash, R.G. 1980. Dissipation Rate of Pesticides from Soils. Chapter 17. IN CREAMS: A Field Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. W.G. Knisel, ed. USDA Conservation Research Report No. 26. 643 pp.

[g] Control of Water Pollution from Cropland, Vol. I, a manual for guideline development, EPA-600/2-75-026a.1

$$\log K_{oc} = 1.00 (\log K_{ow}) - 0.21 \qquad (6\text{-}11)$$

where K_{ow} = octanol-water distribution coefficient ($cm^3\ g^{-1}$)
K_{oc} = organic carbon distribution coefficient ($cm^3\ g^{-1}$)

Carbofuran is a pesticide that exhibits crystalline energy relationships and its apparent distribution coefficient should be estimated using its log K_{ow}, which is 2.44. Substituting into the Karickhoff equation

$$\log K_{oc} = 1.00 (2.44) - 0.21 = 2.23$$

$$K_{oc} = 10^{2.23} = 169.8$$

For a soil with 0.5% organic carbon the K_d of the pesticide is

$$K_d = K_{oc} \frac{\text{percent organic carbon}}{100} \qquad (6\text{-}12)$$

$$K_d = \frac{169.8\ (0.5)}{100} = 0.85$$

This compares to an estimated K_d of 2.68 using the PCMC1 water solubility model. Selected pesticides having properties suitable for use with the octanol water distribution model by Karickhoff are provided in Table 6-21.

DKRATE--degradation rate constants--The processes that contribute to pesticide disappearance in soils are varied and depend on environmental factors as well as chemical properties. Unfortunately, only rarely are process-specific rate constants (e.g., hydrolysis) reported for the soil environment. In most cases, a lumped first-order rate constant is reported. A first order model using a lumped decay rate is used in TFAT. Although such an approximation is imprecise, most modeling efforts follow the same approach and many pesticides appear to behave similarly. For example, Nash (1980) found that disappearance of many compounds was highly correlated to a first order approximation with $r^2 \geq 0.80$.

The dissipation rate of pesticides below the root zone is virtually unknown. Several studies have suggested the rate of dissipation decreases with depth; however, no uniform correction factor was suggested between surface/sub-surface rates. First order dissipation rates for selected pesticides in the root zone are also tabulated in Table 6-21.

UPTKF--plant uptake of pesticides--The plant uptake efficiency factor, or root reflection coefficient (UPTKF) provides for removal of pesticides by plants and is a function of the crop root distribution and the interaction of soil, water, and the pesticide. Several approaches to modeling the uptake of nutrients/pesticides have been proposed ranging from process models that treat the root system as a distribution sink of known density or

TABLE 6-21. OCTANOL WATER DISTRIBUTION COEFFICIENTS (LOG K_{ow}) AND SOIL DEGRADATION RATE CONSTANTS FOR SELECTED CHEMICALS

Chemical Name	Log K_{ow}[b]	Degradation Rate Constant ($days^{-1}$)	Reference
Alachlor	2.78	0.0384	a
Aldicarb	0.70	0.0322 - 0.0116	a
Altosid	2.25		
Atrazine	2.45	0.0149 - 0.0063	a
Benomyl	2.42	0.1486 - 0.0023	a
Bifenox	2.24	0.1420	a
Bromacil	2.02		
Captan	2.35		
Carbaryl	2.56	0.1196 - 0.0768	a
Carbofuran	2.44	0.0768 - 0.0079	a
Chloramben	1.11		
Chlordane	4.47	0.0020 - 0.0007	
Chloroacetic Acid	-0.39		
Chloropropham	3.06	0.0058 - 0.00267	d
Chloropyrifos	4.97		
Cyanazine	2.24	0.0495	c
Dalapon	0.76	0.0462 - 0.0231	d
Dialifor	4.69		
Diazinon	3.02	0.0330 - 0.0067	a
Dicamba	0.48	0.2140 - 0.0197	a
Dichlobenil	2.90	0.0116 - 0.0039	
Dichlorofenthion	5.14		
2,4,-Dichlorophenoxy-acetic Acid	2.81	0.0693 - 0.0231	d
Dichloropropene	1.73		
Dicofol	3.54		
Dinoseb	2.30	0.0462 - 0.0231	d
Diuron	2.81	0.0035 - 0.0014	d
Endrin	3.21		
Fenitrothion	3.36	0.1155 - 0.0578	a
Fluometuron	1.34	0.0231	c
Linuron	2.19	0.0280 - 0.0039	a
Malathion	2.89	02.91 - 0.4152	a
Methomyl	0.69		
Methoxychlor	5.08	0.0046 - 0.0033	a
Methyl Parathion	3.32	0.2207	a
Monolinuron	1.60		
Monuron	2.12	0.0046 - 0.0020	d
MSMA	-3.10		
Nitrofen	3.10		
Parathion	3.81	0.2961 - 0.0046	a

TABLE 6-21. OCTANOL WATER DISTRIBUTION COEFFICIENTS (LOG K_{ow}) AND SOIL DEGRADATION RATE CONSTANTS FOR SELECTED CHEMICALS (CONCLUDED)

Chemical Name	Log K_{ow}[b]	Degradation Rate Constant (days^{-1})	Reference
Permethrin	2.88	0.0396	e
Phorate	2.92	0.0363 - 0.0040	a
Phosalone	4.30		
Phosmet	2.83		
Picloram	0.30	0.0354 - 0.0019	a
Propachlor	1.61	0.0231 - 0.0139	d
Propanil	2.03	0.693 - 0.231	d
Propazine	2.94	0.0035 - 0.0017	d
Propoxur	1.45		
Ronnel	4.88		
Simazine	1.94	0.0539 - 0074	a
Terbacil	1.89		
Terbufos	2.22		
Toxaphene	3.27	0.0046	e
Trifluralin	4.75	0.0956 - 0.0026	a
Zineb	1.78	0.0512	a

[a] Nash, R. G. 1980. Dissipation Rate of Pesticides from Soils. Chapter 17. IN CREAMS: A Field Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. W. G. Knisel, ed. USDA Conservation Research Report No. 26. 643pp.

[b] Smith, C. N. Partition Coefficients (Log K_{ow}) for Selected Chemicals. Athens Environmental Research Laboratory, Athens, GA. Unpublished report, 1981.

[c] Herbicide Handbook of the Weed Science Society of America, 4th ed. 1979.

[d] Control of Water Pollution from Cropland, Vol. I, a manual for guideline development, EPA-600/2-75-026a.

[e] Smith, C. N. and R. F. Carsel. Foliar Washoff of Pesticides (FWOP) Model: Development and Evaluation. Accepted for publishing in Journal of Environmental Science and Health - Part B. Pesticides, Food Contaminants, and Agricultural Wastes, B 19(3), 1984.

strength to empirical approaches that assume a relationship to the transpiration rate. Dejonckheere et al. (1983) reported the mass of uptake into sugar beets for the pesticides aldicarb and thiofanox for three soils (sandy loam, silt loam, and sandy clay loam). Mass removal expressed as a percentage of applied material for aldicarb on sandy loam, silt loam, and clay loam ranged from 0.46-7.14%, 0.68 - 2.32%, and 0.15 - 0.74%, respectively. For thiofanox, 2.78 - 20.22%, 0.81 - 8.70%, and 0.24 2.42% removals were reported for the respective soils. The amount of uptake was higher for sandy soils and increased with available water. Other reviews have suggested ranges from 4 - 20% for removal by plants.

The procedure adopted for TFAT estimates the removal of pesticides by plant uptake based on the assumption that uptake of the pesticide is directly related to the transpiration rate. Sensitivity tests conducted with PRZM indicate an increase in the uptake by plants as the root zone depth increases, and as the partition coefficient decreases. For highly soluble pesticides and for crop root zones less than 120 cm, the model simulates total uptake within the range reported by Dejonckheere et al. For highly soluble pesticides and for crop root zones of greater than 120 cm, values of greater than 20% were simulated. For initial estimates a value of 1.0 for UPTKF is recommended. If more than 20 - 25% of the pesticide is simulated (to be removed by plant uptake), UPTKF should be calibrated to a value less than 1.0.

The value of UPTKF is utilized even if the PLTGRN module is on. The mass flux resulting from the value of UPTRF selected is used as input to the plant translocation model (see Section 6.5).

CORED--thickness of soil column--The user will want to enter a value so that the biologically active portion of the soil is simulated. For field crops and grasses, this will be 100 to 200 cm.

DISP--dispersion coefficient--The dispersion or "smearing out" of the pesticide as it moves down in the soil profile is attributed to a combination of molecular diffusion and dispersion. The transport equations solved in PRZM also produce truncation error leading to a purely mathematical or numerical dispersion. For this reason the DISP parameter must be evaluated in light of both "real" and "numerical" components.

A number of sensitivity simulations using PRZM have been performed to investigate the impact of model parameters other than DISP on the apparent dispersion. From these simulations, the following guidance is offered.

- A spatial step or compartment size of 5.0 cm will mimic observed field effective dispersion quite well and should be used as an initial value.

- No fewer than 30 compartments (parameter NCOM2) should be used.

- The DISP parameter should be set to 0.0 unless field data are available for calibration.

APD, APM, IAPYR--pesticide application--The use of PRZM requires the establishment of a pesticide application procedure. The user should follow the two steps described below in establishing representative application dates:

- establish an application period window covering the range of possible application dates

- adjust the application dates within the window so that application does not occur on a day immediately before, during, or immediately after a rainfall event (pesticides are not normally applied to a field with high moisture content or under conditions where the efficacy would be diminished).

6.4.1.4 Soils Parameters--

The amount of available moisture in the soil is affected by such properties as temperature and humidity, soil texture and structure, organic matter content, and plant characteristics (rooting depth and stage of growth). The moisture remaining in a soil after "gravity drainage" has ceased is known as field capacity. The moisture content in a soil below which plants cannot survive is called the wilting point. The wilting point, which varies among specific soils is influenced by colloidal material and organic matter, but most soils will have a similar wilting point for all common plants.

The PRZM model simulates soil water retention in the context of these bulk soil properties. Drainage of "excess water" is simulated as a simple daily value or as a daily rate. Most specific model parameters can be input directly by the user and some can be internally estimated given certain related soil properties as inputs.

THEFC, THEWP--moisture holding capacity--Field capacity (THEFC) and wilting point (THEWP) are required as user inputs. Often these soil-water properties have been characterized and values can be found from soils data bases. Where such data are not available, one of the three estimation methods given below can be used. Method one requires the textural properties (percent sand, silt, and clay), organic matter content (%), and bulk density (g cm^{-3}) of a specific soil. Method two utilizes a soil texture matrix for estimating soil water content if only the sand (%) and clay (%) contents are known. Method three provides mean field capacity and wilting points if only the soil texture is known.

Method 1 (also done within the code if THFLAG = 1)

The regression equation from Brakensiek and Rawls (1985) to is used estimate the matric water potential for various soils:

$$\Theta_x = a + [b \times SAND(\%)] + (c \times CLAY(\%)] + [d \times ORGANIC\ MATTER(\%)] + [E \times BULK\ DENSITY\ (g\ cm^{-3})] \qquad (6\text{-}12)$$

where Θ_x = water retention $cm^3\ cm^{-3}$ for a given matric potential (field capacity = -0.33 bar and wilting point = -15.0 bar)

a-e = regression coefficients

Step 1. From Table 6-22 find the matric potential for field capacity and wilting point (-0.33 bar and -15.0 bar).

Step 2. For each matric potential, find the regression coefficients (a-e) that are required in the Rawls and Brakensiek equation (e.g., for -0.33 potential, coefficients a-e are 0.3486, -0.0018, 0.0039, 0.0228, and -0.0738).

Step 3. For any given soil (example: Red Bay Sandy Loam where sand (%), 72.90; clay (%), 13.1; organic matter (%), 0.824; and bulk density (g cm^{-3}), 1.70) solve the equation for the -0.33 and -15.0 potential. For this example, THEFC = 0.170, THEWP = 0.090.

Method 2

Use Figure 6-4 for estimating the field capacity and Figure 6-5 for estimating the wilting point of any soil, given the percent sand and clay.

Step 1. Example: Red Bay Sandy Loam (field capacity). Find the percent sand across the bottom of Figure 6-4 (i.e., 73.0)

Step 2. Find the percent clay of the soil along the side of the triangle (i.e., 13.0).

Step 3. Locate the point where the two values intersect on the triangle and read the field capacity, THEFC = 0.17.

Step 4. Follow Steps 2-4 for wilting point using Figure 6-5. THEWP = 0.09.

Method 3

Step 1. Use Table 6-23 to locate the textural class of the soil of choice.

Step 2. After locating the textural class, read the mean field capacity and wilting point potentials ($cm^3\ cm^{-3}$), to the right of the textural class. Example: Sandy loam. The mean field capacity (THEFC) and wilting point (THEWP) potentials are 0.207 and 0.095, respectively.

Guidance for estimating distributional properties for THEFC and THEWP is given in Tables 6-24 and 6-25. These tables show the arithmetic means and coefficients of variation for Hydrologic Groups A, B, C and D soils with depth. Also shown is the type of distribution which is most appropriate.

TABLE 6-22. COEFFICIENTS FOR LINEAR REGRESSION EQUATIONS FOR PREDICTION OF SOIL WATER CONTENTS AT SPECIFIC MATRIC POTENTIALS[a]

Matric Coefficient	Intercept a	Sand (%) b	Clay (%) c	Organic Matter (%) d	Bulk Density ($g\ cm^{-3}$) e	R^2
-0.20	0.4180	-0.0021	0.0035	0.0232	-0.0859	0.75
-0.33	0.3486	-0.0018	0.0039	0.0228	-0.0738	0.78
-0.60	0.2819	-0.0014	0.0042	0.0216	-0.0612	0.78
-1.0	0.2352	-0.0012	0.0043	0.0202	-0.0517	0.76
-2.0	0.1837	-0.0009	0.0044	0.0181	-0.0407	0.74
-4.0	0.1426	0.0007	0.0045	0.0160	-0.0315	0.71
-7.0	0.1155	-0.0005	0.0045	0.0143	-0.0253	0.69
-10.0	0.1005	-0.0004	0.0044	0.0133	-0.0218	0.67
-15.0	0.0854	-0.0004	0.0044	0.0122	-0.0182	0.66

[a] Rawls, W. J., U.S. Department of Agriculture, Agricultural Research Service, Beltsville, MD. Personal Communication.

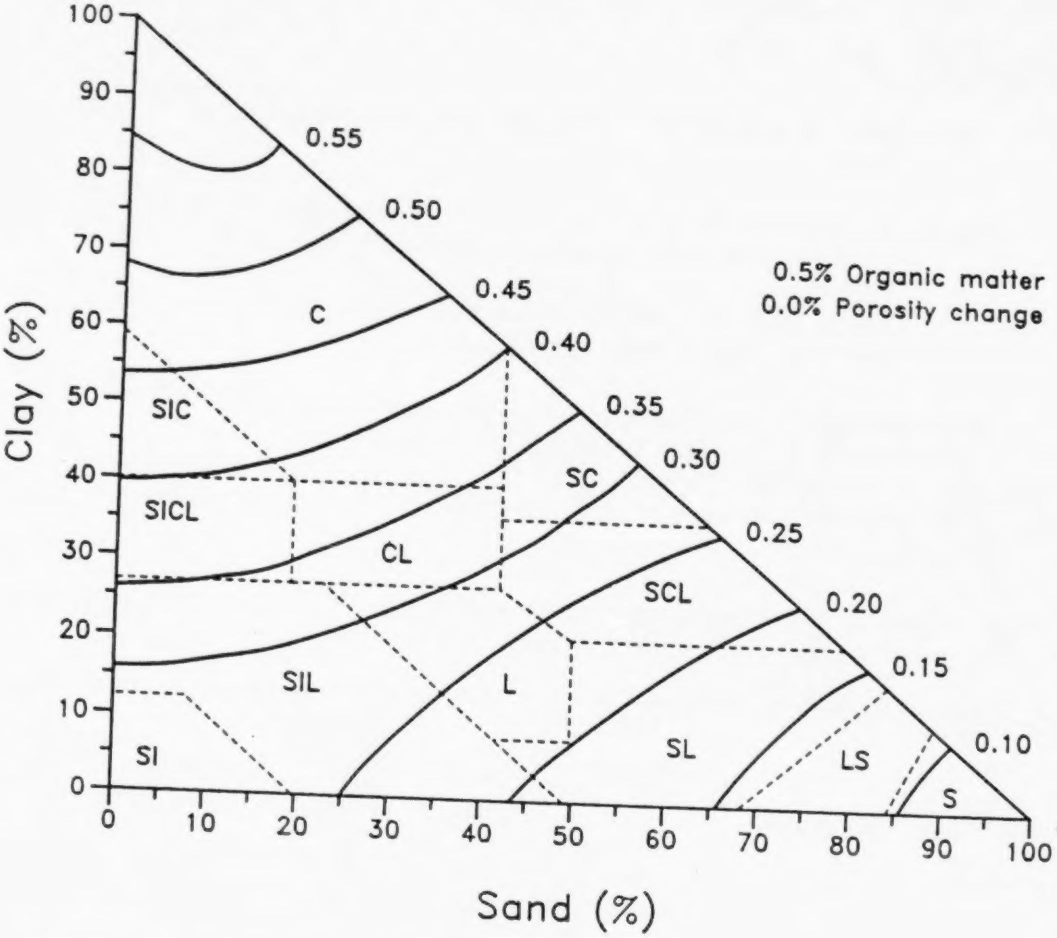

Figure 6.4 1/3-Bar soil moisture by volume. (Provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Service, Beltsville, Maryland.)

Jury (1985) indicates overall CV for wilting point water content (15 bar tension) to be lower, at 24 percent. He also indicates that the most appropriate distribution for static soil properties such as these is the normal.

Correlation coefficients between fixed capacity and wilting point have moderate to high values ranging from 0.64 to 0.85 (Carsel et al. 1988).

BD--bulk density and field saturation--Soil bulk density (BD) is required in the basic chemical transport equations of TFAT and is also used to estimate moisture saturation values. Values for BD can be input directly. When such data are not available for the site of interest, methods have been developed for their estimation. Two methods are provided for estimating BD of various soils. Method one requires the textural properties (percent sand, clay, and organic matter). Method two uses mean bulk density values if only the soil texture is known. The following steps provide procedures for estimating bulk density.

Method 1 (Also done within the code if BDFLAG = 1)

A procedure from Rawls (1983) is used to estimate bulk density for any given soil, provided the percent sand, clay, and organic matter contents are known. Example: Marlboro fine sandy loam--sand 80.0%, clay 5.0%, and organic matter 0.871%. Using the following equation:

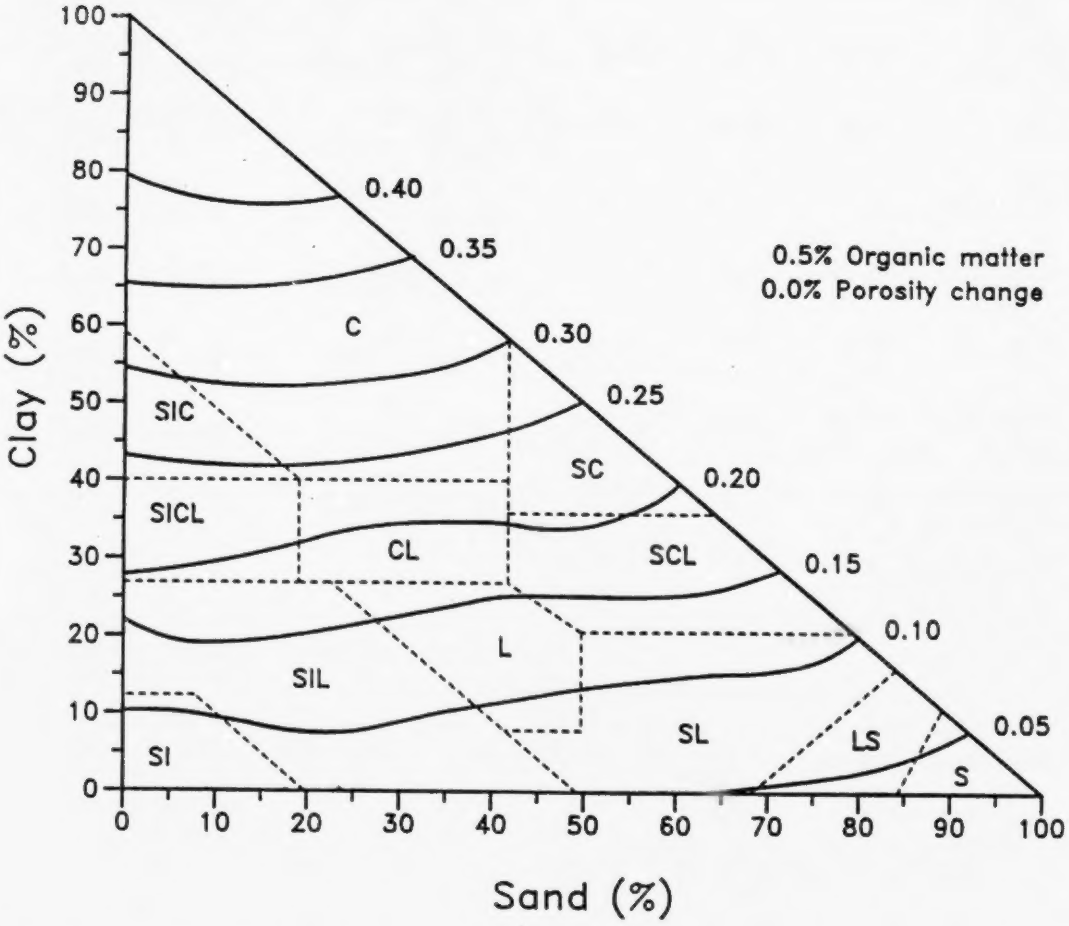

Figure 6.5 15-Bar soil moisture by volume. (Provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Service, Beltsville, Maryland.)

TABLE 6-23. HYDROLOGIC PROPERTIES BY SOIL TEXTURE[a]

Texture Class	Range of Textural Properties (Percent)			Water Retained at -0.33 Bar Tension $cm^3\ cm^{-3}$	Water Retained at -15.0 Bar Tension $cm^3\ cm^{-3}$
	Sand	Silt	Clay		
Sand	85-100	0-15	0-10	0.091[b] (0.018 - 0.164)[c]	0.033[b] (0.007 - 0.059)[c]
Loamy Sand	70-90	0-30	0-15	0.125 (0.060 - 0.190)	0.055 (0.019 - 0.091)
Sandy Loam	45-85	0-50	0-20	0.207 (0.126 - 0.288)	0.095 (0.031 - 0.159)
Loam	25-50	28-50	8-28	0.270 (0.195 - 0.345)	0.117 (0.069 - 0.165)
Silt Loam	0-50	50-100	0-28	0.330 (0.258 - 0.402)	0.133 (0.078 - 0.188)
Sandy Clay Loam	45-80	0-28	20-35	0.257 (0.186 - 0.324)	0.148 (0.085 - 0.211)
Clay Loam	20-45	15-55	28-50	0.318 (0.250 - 0.386)	0.197 (0.115 - 0.279)
Silty Clay Loam	0-20	40-73	28-40	0.366 (0.304 - 0.428)	0.208 (0.138 - 0.278)
Sandy Clay	45-65	0-20	35-55	0.339 (0.245 - 0.433)	0.239 (0.162 - 0.316)
Silty Clay	0-20	40-60	40-60	0.387 (0.332 - 0.442)	0.250 (0.193 - 0.307)
Clay	0-45	0-40	40-100	0.396 (0.326 - 0.466)	0.272 (0.208 - 0.336)

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[a] Rawls, W. J., D. L. Brakensiek, and K. E. Saxton. Estimation of Soil Water Properties. Transactions ASAE Paper No. 81-2510, pp. 1316 - 1320. 1982.

[b] Mean value.

[c] One standard deviation about the mean.

TABLE 6-24. DESCRIPTIVE STATISTICS AND DISTRIBUTION MODEL FOR FIELD CAPACITY (PERCENT BY VOLUME)

Stratum (m)	Sample Size	Original Data				Distribution Model		
		Mean	Median	s.d.	cv (%)	Transform	Mean	s.d.
Class A								
0.0-0.3	52	11.8	9.4	9.2	78	ln	2.25	0.65
0.3-0.6	50	9.6	8.1	7.9	82	ln	1.99	0.73
0.6-0.9	42	7.3	5.9	5.8	79	ln	1.73	0.73
0.9-1.2	39	7.1	5.8	5.0	70	ln	1.73	0.71
Class B								
0.0-0.3	456	19.5	19.1	8.3	42	s_U	0.316	0.13
0.3-0.6	454	18.8	18.8	7.4	39	s_U	0.311	0.12
0.6-0.9	435	18.7	18.7	7.1	39	s_U	0.298	0.11
0.9-1.2	373	17.5	17.5	7.6	43	s_U	0.288	0.12
Class C								
0.0-0.3	371	22.4	22.5	7.8	35	s_U	0.363	0.12
0.3-0.6	362	22.8	23.2	7.8	34	s_U	0.369	0.12
0.6-0.9	336	22.7	22.9	8.6	38	s_U	0.368	0.13
0.9-1.2	290	22.2	21.3	8.9	40	s_U	0.359	0.13
Class D								
0.0-0.3	230	24.1	24.2	9.1	38	s_U	0.387	0.14
0.3-0.6	208	26.1	26.3	9.3	36	s_U	0.419	0.14
0.6-0.9	178	25.0	25.6	8.2	33	s_U	0.403	0.13
0.9-1.2	146	24.1	24.4	8.1	33	s_U	0.390	0.12

s.d. = standard deviation
cv = coefficient of variation

Source: Carsel et al. (1988)

TABLE 6-25. DESCRIPTIVE STATISTICS AND DISTRIBUTION MODEL FOR WILTING POINT (PERCENT BY VOLUME)

Stratum (m)	Sample Size	Original Data			cv (%)	Distribution Model		
		Mean	Median	s.d.		Transform	Mean	s.d.
Class A								
0.0-0.3	118	4.1	3.1	3.4	82	ln	1.83	0.64
0.3-0.6	119	3.2	2.3	2.4	75	ln	0.915	0.71
0.6-0.9	113	2.9	2.1	2.3	81	s_B	3.32	0.88
0.9-1.2	105	2.6	1.9	2.3	87	s_B	3.43	0.92
Class B								
0.0-0.3	880	9.0	8.7	4.0	45	s_U	0.150	0.066
0.3-0.6	883	9.4	9.3	4.3	46	s_U	0.156	0.071
0.6-0.9	866	9.1	8.9	4.4	48	s_U	0.151	0.072
0.6-1.2	866	8.6	8.4	4.6	53	s_U	0.143	0.076
Class C								
0.3-0.3	678	10.8	10.4	5.1	48	s_U	1.63	0.62
0.3-0.6	677	12.2	12.1	5.6	46	s_U	0.202	0.091
0.6-0.9	652	12.2	11.9	6.0	49	s_U	0.201	0.096
0.9-1.2	582	11.8	11.5	5.7	48	s_U	0.194	0.092
Class D								
0.0-0.3	495	14.6	13.8	7.6	52	s_U	1.26	0.76
0.3-0.6	485	16.9	17.0	7.3	43	s_U	0.277	0.12
0.6-0.9	437	16.6	16.3	7.4	45	s_U	0.271	0.12
0.9-1.2	401	15.7	15.1	7.6	48	s_U	0.257	0.12

s.d. = standard deviation
cv = coefficient of variation

Source: Carsel et al. (1988)

$$BD = \frac{100.0}{\frac{\%OM}{OMBD} + \frac{100.0 - \%OM}{MBD}} \qquad (6\text{-}13)$$

where BD = soil bulk density, g cm^{-3}
OM = organic matter content of soil, %
OMBD = organic matter bulk density of soil, g cm^{-3} = 0.224
MBD = mineral bulk density, g cm^{-3}

NOTE: MBD must be entered if BDFLAG = 1.

Step 1. Locate the percent sand (80.0) along the bottom of Figure 6-6.

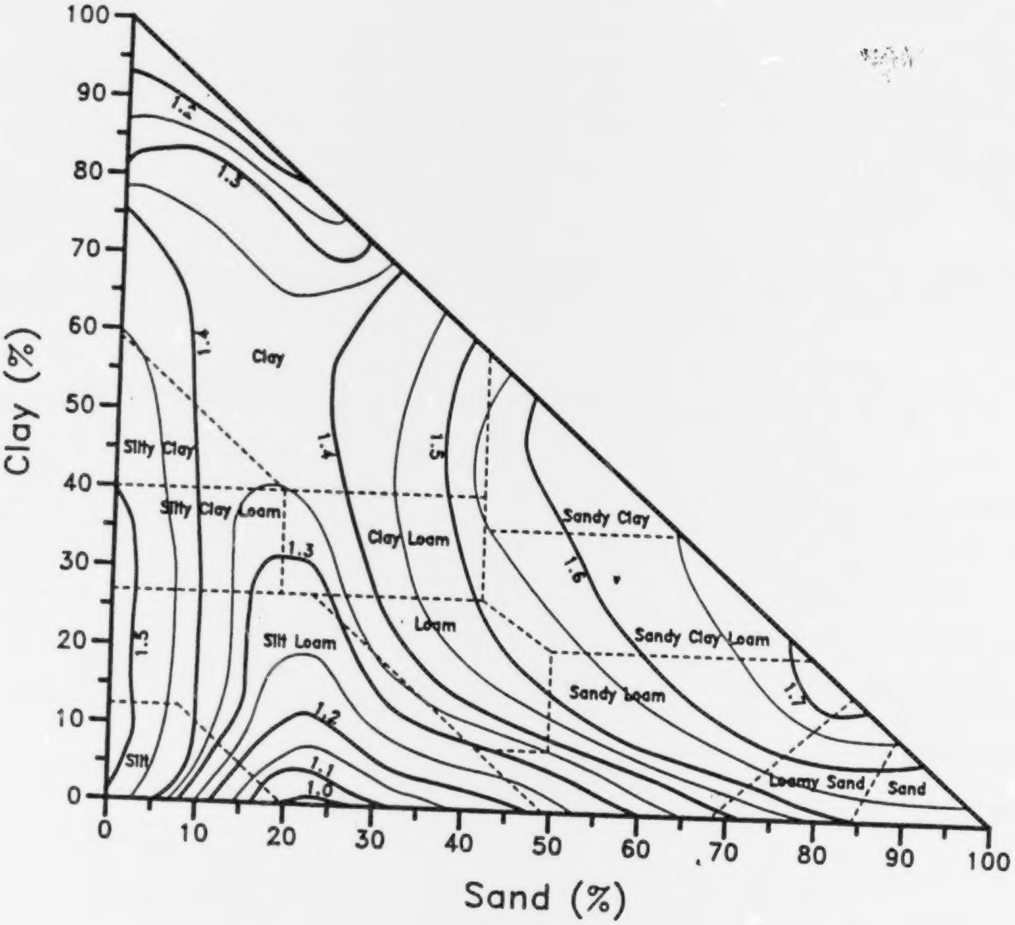

Figure 6.6 Mineral bulk density (g cm^{-3}). (Provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Science, Beltsville, Maryland.)

Step 2. Locate the percent clay (5.0) along the side of Figure 6-6.

Step 3. Locate the intersection point of the two values and read the mineral bulk density (1.55).

Step 4. Solve the Rawls equation for BD (e.g., 1.47).

Method 2

Step 1. Use Table 6-26 to locate the textural classification of the soil.

Step 2. Read mean bulk density for the general soil texture. Example: Sandy loam. The mean bulk density is 1.49 g cm^{-3}.

Table 6-27 shows distributional properties of bulk density information. The information given is categorized by Hydrologic Soil Group (A, B, C, D). The most appropriate distribution for this property is the normal (Jury 1985). Jury indicates slightly lower CVs, on the order of 9 percent.

OC--percent of soil organic matter--Guidance on estimating percent organic matter is found in Table 6-28. Information is categorized by Hydrologic Soil Group and by depth. Also shown are coefficients of

TABLE 6-26. MEAN BULK DENSITY (g cm^{-3}) FOR FIVE SOIL TEXTURAL CLASSIFICATIONS[a]

Soil Texture	Mean Value	Range Reported
Silt Loams	1.32	0.86 - 1.67
Clay and Clay Loams	1.30	0.94 - 1.54
Sandy Loams	1.49	1.25 - 1.76
Gravelly Silt Loams	1.22	1.02 - 1.58
Loams	1.42	1.16 - 1.58
All Soils	1.35	0.86 - 1.76

[a] Baes, C. F., III and R. D. Sharp. 1983. A Proposal for Estimation of Soil Leaching Constants for Use in Assessment Models. J. Environ. Qual. 12(1): 17-28.

TABLE 6-27. DESCRIPTIVE STATISTICS FOR BULK DENSITY (9 CM^{-3})

Stratum (m)	Sample Size	Mean	Median	s.d.	cv (%)
Class A					
0.0-0.3	40	1.45	1.53	0.24	16.2
0.3-0.6	44	1.50	1.56	0.23	15.6
0.6-0.9	38	1.57	1.55	0.16	10.5
0.9-1.2	34	1.58	1.59	0.13	8.4
Class B					
0.0-0.3	459	1.44	1.45	0.19	13.5
0.3-0.6	457	1.51	1.53	0.19	12.2
0.6-0.9	438	1.56	1.57	0.19	12.3
0.9-1.2	384	1.60	1.60	0.21	12.9
Class C					
0.0-0.3	398	1.46	1.48	0.22	15.0
0.3-0.6	395	1.58	1.59	0.23	14.5
0.6-0.9	371	1.64	1.65	0.23	14.2
0.9-1.2	326	1.67	1.68	0.23	14.0
Class D					
0.0-0.3	259	1.52	1.53	0.24	15.9
0.3-0.6	244	1.63	1.66	0.26	16.0
0.6-0.9	214	1.67	1.72	0.27	16.3
0.9-1.2	180	1.65	1.72	0.28	17.0

s.d. = standard deviation
cv = coefficient of variation

Source: Carsel et al. (1988)

variation for each soil group and depth. Carsel et al. (1988) determined that the Johnson SB distribution provides the best fit to this data.

Rao and Wagenet (1985) and Nielsen et al. (1983) have reported that these values are often normally distributed. Carsel et al. (1988) have noted that organic carbon is weakly correlated with field capacity and wilting point water content with correlation coefficients ranging from 0.1 to 0.74. Strength of correlation decreases with depth.

AD--soil water drainage rate (for HSWZT = 1)--The HSWZT flag indicates which drainage model is invoked for simulating the movement of recharging water. Drainage model 1 (HSWZT = 0) is for freely draining soils; drainage model 2 (HSWZT = 1) is for more poorly drained soils. For soils with infiltration rates of more than 0.38 cm hr^{-1} (associated with SCS hydrologic soils groups A, B, and some C), setting HSWZT = 0 is recommended. For soils with infiltration rates of less than 0.38 cm hr^{-1} (associated with groups D and some C) setting HSWZT = 1 is recommended.

The drainage rate parameter (AD), required when HSWZT = 1, is an empirical constant and dependent on both soil type and the number of compartments to be simulated. Although there is limited experience using this option, an analysis was performed to determine the best value for AD

TABLE 6-28. DESCRIPTIVE STATISTICS AND DISTRIBUTION MODEL FOR ORGANIC MATTER (PERCENT BY WEIGHT)

Stratum (m)	Sample Size	Original Data				Distribution Model[a]	
		Mean	Median	s.d.	C_{var} (%)	Mean	s.d.
Class A							
0.0-0.3	162	0.86	0.62	0.79	92	-4.53	0.96
0.3-0.6	162	0.29	0.19	0.34	114	-5.72	0.91
0.6-0.9	151	0.15	0.10	0.14	94	-6.33	0.83
0.9-1.2	134	0.11	0.07	0.11	104	-6.72	0.87
Class B							
0.0-0.3	1135	1.3	1.1	0.87	68	-4.02	0.76
0.3-0.6	1120	0.50	0.40	0.40	83	-5.04	0.77
0.6-0.9	1090	0.27	0.22	0.23	84	-5.65	0.75
0.9-1.2	1001	0.18	0.14	0.16	87	-6.10	0.78
Class C							
0.0-0.3	838	1.45	1.15	1.12	77	-3.95	0.79
0.3-0.6	822	0.53	0.39	0.61	114	-5.08	0.84
0.3-0.9	780	0.28	0.22	0.27	96	-5.67	0.83
0.9-1.2	672	0.20	0.15	0.21	104	-6.03	0.88
Class D							
0.0-0.3	638	1.34	1.15	0.87	66	-4.01	0.73
0.3-0.6	617	0.65	0.53	0.52	80	-4.79	0.78
0.6-0.9	558	0.41	0.32	0.34	84	-5.29	0.82
0.9-1.2	493	0.29	0.22	0.31	105	-5.65	0.86

s.d. = standard deviation
CV = coefficient of variation

[a] Johnson s_B transformation is used for all cases in this table

Source: Carsel et al. (1988)

over a range of soil types on which agricultural crops are commonly grown. Each of three soil types was tested with a constant soil profile depth (125 cm). The profile was divided into a variable number of compartments and the optimum value of AD for each soil/compartment combination was obtained.

The analysis was performed by comparing the storage of water in the soil profile following the infiltration output from SUMATRA-1 (van Genuchten 1978). This model was used as "truth" because field data were lacking and SUMATRA-1 is theoretically rigorous. The amount of water moving out of the profile changed by only 1 - 2% over the range of compartments tested (15 - 40) for the three soils evaluated. Calibrating PRZM by comparison was accomplished and estimates of AD calculated. Suggested values of AD for clay loam, loamy sand, and sand as a function of the number of compartments are given in Figure 6-7.

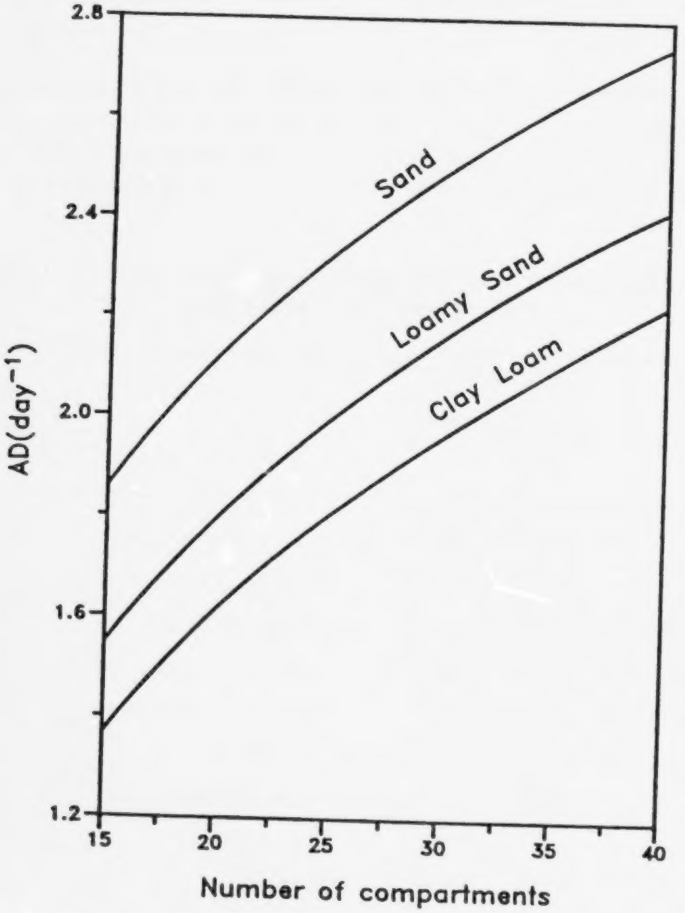

Figure 6.7 Estimation of drainage rate AD (day^{-1}) versus number of compartments.

6.4.2 Infiltration and Ponding

KSAT--saturated hydraulic conductivity--This parameter represents the limiting infiltration rate when the soil column is saturated and suction pressure is not longer important. KSAT depends upon soil mineralogy, texture, and degree of compaction. Ranges of values for various unconsolidated materials are shown in Table 6-29. Note that these values are given in ms^{-1} whereas TEEAM requires units of cm hr^{-1}. KSAT has also been correlated with SCS Hydrologic Soil Groups (Brakensiek and Rawls 1983); ranges of values for each soil group are shown in Table 6-30.

For Monte Carlo simulation, it has often been observed that the distribution of hydraulic conductivities in both surface soils and groundwater aquifers is approximately log-normal (Freeze 1975; Willardson and Hurst 1965). Jury (1985) gives values for the coefficient of variation of 120 percent. Table 6-31 gives distributional properties for various soil textures.

HFPOND--suction parameter--HFPOND represents water movement due to suction in unsaturated soils, and has units of length (cm). As in the case of KSAT, HF pond has been correlated with SCS Hydrologic Soil Groups (Brakensiek and Rawls 1983); ranges of values for each soil group are shown in Table 6-29.

TABLE 6-29. REPRESENTATIVE SATURATED HYDRAULIC CONDUCTIVITY RANGES FOR SEDIMENTARY MATERIALS

Material	Saturated Hydraulic Conductivity (ms^{-1})	Material	Saturated Hydraulic Conductivity (ms^{-1})
Clay	10^{-12} - 10^{-9}	Very fine sand	10^{-7} - 10^{-4}
Silty clay	10^{-12} - 10^{-9}	Find sand	10^{-6} - 10^{-3}
Sandy clay	10^{-11} - 10^{-8}	Medium sand	10^{-5} - 10^{-3}
Silty clay loam	10^{-10} - 10^{-7}	Coarse sand	10^{-5} - 10^{-2}
Sandy loam sand	10^{-9} - 10^{-6}	Gravel and sand	10^{-5} - 10^{-2}
Silt	10^{-9} - 10^{-6}	Gravel	10^{-5} - 10^{-2}
Silt loam	10^{-9} - 10^{-6}	Sandstone	10^{-6} - 10^{-3}
Loam	10^{-9} - 10^{-6}	Limestone*	10^{-7} - 10^{-4}
Sandy loam	10^{-8} - 10^{-7}	Shale	10^{-7} - 10^{-4}

* Excluding cavernous limestone.
Source: Adapted from Todd (1970).

TABLE 6-30. VALUES OF GREEN-AMPT PARAMETERS FOR SCS HYDROLOGIC SOIL GROUPS

SCS Hydrologic Soil Group	Saturated Hydraulic Conductivity KS (cm/hr)	Suction Parameter HF (cm)
A	1.0 - 10.0	10
B	.60 - 1.0	10 - 20
C	.20 - .60	15 - 10
D	.005 - .20	20 - 150

Source: Adapted from Brakensiek and Rawls (1983).

TC--time of concentration for runoff--This parameter represents the time it takes for runoff to travel from the hydraulically most distant part of a catchment (in this case, habitat) to the point of discharge. In hydrograph analysis, TC is the time from the end of rainfall excess to the point on the falling limb of the hydrograph where the recession curve begins (Mockus 1972). TC is a physical characteristic of the catchment, and will depend upon the shape of the catchment, ground slope, drainage density, and surface roughness. A number of methods for estimating TC are described in the Soil Conservation Service Hydrology Handbook (Mockus 1972). The following empirical equation described in the SCS Handbook can be used for areas of less than 2000 acres:

$$TC = \frac{1.7\ell^{0.8}(S + 1)^{0.7}}{1900\ Y^{0.5}} \qquad (6\text{-}14)$$

where

TC = Time of concentration (hours)
ℓ = Hydraulic length of the catchment (ft)
S = Watershed retention parameter
$= \frac{1000}{CN} - 10$
CN = SCS runoff curve number for the catchment
Y = Average catchment slope (percent)

Other guidance for estimating TC can be obtained from local flood control districts and Soil Conservation Service Offices.

TABLE 6-31. DESCRIPTIVE STATISTICS FOR SATURATED HYDRAULIC CONDUCTIVITY (KSAT) (cm hr^{-1})

Soil Type	Hydraulic Conductivity (KSAT)			
	$\bar{x}$	s	CV	n
Clay**	0.20	0.42	210.3	114
Clay Loam	0.26	0.70	267.2	345
Loam	1.04	1.82	174.6	735
Loamy Sand	14.59	11.36	77.9	315
Silt	0.25	0.33	129.9	88
Silt Loam	0.45	1.23	275.1	1093
Silty Clay	0.02	0.11	453.3	126
Silty Clay Loam	0.07	0.19	288.7	592
Sand	29.70	15.60	52.4	246
Sandy Clay	0.12	0.28	234.1	46
Sandy Clay Loam	1.31	2.74	208.6	214
Sandy Loam	4.42	5.63	127.0	1183

* n = Sample size, $\bar{x}$ = Mean, s = Standard deviation, CV = Coefficient of variation (percent)

** Agricultural soil, less than 60 percent clay

Source: Carsel and Parrish (1988).

ARAIN, BRAIN--constants in the rainfall-duration curve--ARAIN and BRAIN are used to relate rainfall amount to rainfall duration. These parameters depend upon storm patterns, topography, and season. Estimates of these constants can be obtained from rainfall-duration data by plotting the logarithms of rainfall amount (cm) against the logarithms of duration (hours). BRAIN can then be estimated as the slope of the best fit line to these data, while ARAIN can be estimated as the inverse logarithm of the intercept. Dean (1979) found the values of these parameters shown below for winter and summer storms in Watkinsville, GA:

Season	ARAIN	BRAIN	R2
Winter	3.25	1.47	0.599
Summer	1.61	1.30	0.525

For instance, for a typical summer storm at Watkinsville, if the depth is 1.5 inches (3.81 cm), the average duration is

$$\begin{aligned} DUR &= 1.61\ (3.81)^{1.30} \\ &= 9.2 \text{ hours} \end{aligned}$$

These values are probably representative for convective-type summer storms and frontal-type winter storms occurring in most parts of the U.S. east of the Rocky Mountains.

6.4.3 Volatilization and Pond Chemistry

DAIR--vapor phase diffusion coefficient--The diffusion coefficient is defined by Fick's first law as the proportionality between the chemical flux and the spatial gradient of concentration. Although in theory DAIR will be chemical and temperature dependent, Jury et al. (1983) found that the vapor diffusion coefficient showed little variation among pesticides and recommended a value of 4,300 cm^2 day^{-1} for all pesticides. Thibodeaux and Scott (1985) calculated values ranging from 3900 to 7800 cm^{2}day^{-1} for 12 benchmark chemicals exhibiting a broad spectrum of characteristics. Included among these were DDT and chlorpyrifos with diffusion coefficients of 4000 and 3900 cm^2 day^{-1} respectively. Diffusion coefficients can also be estimated as a function of temperature and molecule size using techniques described by Lyman et al. (1982).

DWAT--molecular diffusion coefficient in water--DWAT represents the rate of diffusion of dissolved chemical through water, and is a function of temperature, viscosity, and molecule size. Water diffusion coefficients are generally on the order of four orders of magnitude smaller than vapor diffusion coefficients. Lyman et al. (1982) present a number of estimation methods but recommend the Hayduk-Laudie equation due to its simplicity and relative accuracy:

$$DWAT = \frac{11.46^{-5}}{(n_w)^{1.14}\ (V_B)^{0.589}} \qquad (6\text{-}15)$$

where

n_w = the viscosity of water (centi-poise)
V_B = the Lebas moal volume of the chemical (cm^3 molecule^{-1})

V_B can be estimated as described by Lyman et al. (1982).

KH--Henry's law constant--Henry's law constant, used here in dimensionless form, relates the equilibrium concentration of pesticide vapor to the concentration of the water dissolved phase. Table 6-32 is a compilation of a number of experimentally determined values of KH for various chemicals. If KH has not been measured for a chemical, it can be estimated as the ratio of the saturated vapor density to the solubility in water:

$$KH = \frac{C_v}{C_L} \tag{6-16}$$

where

C_v = saturated vapor density for the pesticide (mg ℓ^{-1})
C_L = water solubility of the pesticide (mg ℓ^{-1})

KDPOND--decay rate constant for pesticide in ponds--KDPOND is a lumped first order rate constant used to represent chemical transformation processes such as microbial degradation and hydrolysis. This term does not represent volatilization or infiltration losses since these processes are modeled explicitly by the TFAT ponding algorithm. At this time, there are few data on decay of chemicals in ponds, and KDPOND should only be used to model losses which cannot be explained by volatilization or infiltration.

6.4.4 Granular Formulations

GKWET and GKDRY--wet and dry decay rate constants for granular pesticide--GKWET and GKDRY are rate constants which determine the release of pesticide from granules applied to the soil surface, and have units of days^{-1}. The values of these parameters will vary depending upon the chemical properties of the pesticide and the structure of the granules. As an initial guide for these parameters, Table 6-33 lists overall measured rate constants for granules under various lab and field conditions. GKWET is the rate constant for granules immersed in water, and reflects moisture-dependent processes such as diffusion, leaching, and biodegradation. This parameter can be estimated from plots of immersed granule pesticide concentration against time. If the half-life of pesticide in immersed granules is known, the wet rate constant can be estimated as follows:

$$GKWET = \frac{.693}{t_{1/2}} \tag{6-17}$$

where $t_{1/2}$ is the time in days at which 50 percent of the pesticide mass has been released from the granules. Half-lives and decay rate constants for water-immersed granules can often be obtained from the pesticide manufacturer, since laboratory immersion tests are commonly performed on new granule formulations. The dry rate constant GKDRY is a lumped parameter which is intended to reflect release processes occurring when granules are dry, such as volatilization. Volatilization rate constants can be estimated

TABLE 6-32. ESTIMATED VALUES OF HENRY'S CONSTANT FOR SELECTED PESTICIDES

Compound	Henry's constant (dimensionless)	Ref.
Alachlor	1.3E-06	A
Aldrin	6.3E-04	D
Anthracene	4.4E-05	D
Atrazine	2.5E-07	A
Bentazon	2.0E-10	A
Bromacil	3.7E-08	C
Butylate	3.3E-03	A
Carbaryl	1.1E-05	A
Carbofuran	1.4E-07	A
Chlopyrifos	1.2E-03	A
Chrysene	4.7E-05	D
Cyanazine	1.2E-10	A
DDT	2.0E-03	C
Diazinon	5.0E-05	C
Dicamba	3.3E-08	A
Dieldrin	6.7E-04	C
Diuron	5.4E-08	C
Endrin	1.8E-05	D
EPTC	5.9E-04	C
Ethoprophos	6.0E-06	C
Fenitrothion	6.0E-06	B
Fonofos	2.1E-04	A
Heptachlor	1.7E-02	D
Lindane	1.3E-04	B
Linuron	2.7E-06	A
Malathion	2.4E-06	B
Methomyl	4.3E-08	A
Methyl Parathion	4.4E-06	A
Metolachlor	3.8E-07	A
Metribuzin	9.8E-08	A
Monuron	7.6E-09	C
Napropamide	7.9E-07	C
Parathion	6.1E-06	C
Permethrin	6.2E-05	A
Picloram	1.9E-08	B
Prometryne	5.6E-07	C
Simazine	1.3E-08	A
Terbufos	1.1E-03	A
Toxaphene	2.3E+00	A
Triallate	7.9E-04	C
Trichlorfon	1.5E-09	B
Trifluralin	6.7E-03	A
2, 4-D (acid)	5.6E-09	A
2, 4, 5-T (acid)	7.2E-09	B

References:

A	Donigian et al. (1986)	C	Jury et al. (1984)
B	Spencer et al. (1984)	D	Schnoor et al. (1987)

TABLE 6-33. MEASURED RATE CONSTANTS FOR RELEASE OF PESTICIDES FROM GRANULES

Pesticide	ConditionsConstant (days^{-1})	Source	
Chlorpyrifos	Incorporated in open sand, 5% moisture	.032	Chapman and Chapman (1986)
	Incorporated in closed container of sand, 5% moisture	.014	Chapman and Chapman (1986)
	Incorporated in open container of muck, 65% moisture	.016	Chapman and Chapman (1986)
	Incorporated in closed container of muck, 65% moisture	.018	Chapman and Chapman (1986)
	Incorporated in field muck	.038-.046	Davis and Kuhr (1976)
	Incorporated in loam, lab test	.059-.096	Tashiro and Kuhr (1978)
	Incorporated in loam, field test	.008	Getzin (1985)
	Surface application, field test	.018	Getzin (1985)
Carbofuran	450 g of pesticide in 300-500) m lignin granules, immersed in water	.63	Wilkins (1984)
	450 g of pesticide in 500-1000)m lignin granules, immersed in water	.23	Wilkins (1984)
	450 g of pesticide in 1000-1400)m lignin granules, immersed in water	.086	Wilkins (1984)

by comparing release rates in open and closed containers (Chapman and Chapman 1986). Release rates in open containers will include volatilization of pesticide vapor, whereas volatilized vapor will be trapped in closed containers.

6.4.5 Soil Surface Temperature Regression Coefficients

In order to estimate soil surface temperatures from air temperatures from the equation

$$T_s = A + BT_a \qquad (6\text{-}18)$$

the regression coefficients A and B must be given values. Guidance is provided from two data sets in the literature. Baver et al. (1972) present the data of Smith (1932), which show the monthly variation of air and surface soil temperatures at a 6-inch depth. Representative data are also given by Gibbs et al. (1980). The data of Gibbs et al. represent 10-year averages (1969-1978) for plots having bare soil and sod cover as surface treatments. Regression of soil temperatures on air temperatures give the coefficients shown in Table 6-34. Coefficients of determination (R^2) indicate an excellent linear fit for both data sets. Intercept (A) values range from 0.6° to 14.5°C, whereas slope values (B) ranges from 0.82 to 1.5. Warmer surface soil temperatures are associated with warmer average air temperatures. Therefore, higher values of the intercept should be used in areas having higher air temperatures. The effect of a cover on the soil is to damp temperatures fluctuations by providing insulation. Therefore, soil surface temperatures will be warmer under a vegetative cover when air temperatures are cold and cooler when air temperatures are warm. Wetter soils will tend to be less subject to variation than dry soils because water increases the soil's heat capacity and thermal conductivity (Baver et al. 1972). Therefore, higher-valued intercepts and slopes for the regression equation would be more appropriate for better-insulated soils.

6.5 PLTGRN PARAMETERS

The plant growth module (PLTGRN) of TEEAM is an adaption of the EPIC plant growth model (Williams et al. 1988). The parameters to define plant growth can, for the most part, be estimated using the guidance provided in the EPIC documentation (Williams et al. 1987). Typical ranges (as suggested by Williams et al. 1987) for these plant parameters are presented in Table 6-35.

The EPIC documentation includes the parameters for defining 69 crop types. Parameters for defining 11 of these crop types are provided in Table 6-36. The values listed in this table are useful starting values. When used in a specific modeling scenario, it is recommended that the values be adjusted (calibrated) to represent observed conditions.

TABLE 6-34. EXAMPLE REGRESSIONS OF SURFACE SOIL TEMPERATURE ON AIR TEMPERATURE

Location	A	B	R^2	$\bar{T}_a$
California	14.5	1.5	0.97	44
Geneva, NY				
Bare Soil	0.6	1.1	0.98	13
Soil Cover	1.6	0.82	0.97	13

6.6 PLTRNS MODULE

The required inputs for the plant translocation are few, and with the exception of a few coefficients, can be derived from readily available information. Generalized discussions and review of much of the available literature on adsorption and translocation of pesticides (herbicides) in plants can be found in Ashton and Crafts (1981).

6.6.1 RW--Root Reflection Coefficient

Nash (1974) reviewed the literature on uptake of pesticides by plants to that date. He concluded that, below molecular weights of 500, plants tend not to discriminate between organic molecules except on the basis of polarity, and the single most important factor in determining uptake appears to be solubility. Therefore, one might suspect that the reflection coefficient would vary proportionately with solubility or inversely with K_{ow}. This observed effect may be due to decreased availability of dissolved phase chemical due to adsorption onto soil materials. McFarlane et al. (1987) concluded that the uptake rates of bromacil, phenol, and nitrobenzene were quite different, even though their K_{ow} values are comparable (1.49 to 2.02). Increases in the rate of transpiration stimulated uptake of bromacil and nitrobenzene, (indicating the utility of the transpiration-based uptake model) but had no effect on the uptake of phenol. However, the log of the average rate constant for uptake was highly inversely correlated (R^2=0.98) with the K_{ow} of the chemical. This suggests that chemicals with low K_{ow} should have reflection coefficients closer to unity and chemicals with higher K_{ow} would have coefficients closer to zero. This is consistent with chromatographic theory of transport of organic chemicals in media containing water and an immobile organic phase and with the observations of Briggs et al. (1983). More discussion for this parameter can be found under the UKTKF parameter (Section 6.4.1.3).

6.6.2 LAMDA--Degradation Rate of the Contaminant Within the Plant

Briggs et al. (1982) measured the degradation of some O-methylcarbamoyloxime chemicals and substituted phenylureas in plant shoots. First order degradation constants (day^{-1}) were reported. These values are shown below:

TABLE 6-35. PLANT GROWTH PARAMETERS, TYPICAL RANGES

Variable	Description	Units	Typical Range
PHU	Potential heat units	°C-day	a
BE	Biomass-energy ratio	kg/ha MJ	10-50
FGK	Harvest index	decimal	0.01-0.95
TOPT	Optimal temperature	°C	10-30
TBASE	Base temperature (minimum temperature for plant growth)	°C	0-12
LAIMX	Maximum leaf area index	decimal	0.5-10.0
FLAI	Fraction of growing season where leaf area starts to decline	decimal	0.4-0.99
KHGT	Plant height increase rate	m day^{-1}	b
HGTMX	Maximum crop height	m	0.1-3.0
RZ	Maximum root depth	cm	50-300

[a] Can be estimated for the plant as the sum of the average daily temperature minus the plant base temperature (TBASE) over the period from planting to harvest.

[b] Best estimate is maximum height divided by length of period from emergence to crop maturity.

Chemical	Rate (day^{-1})
Oxamyl O-Methylcarbamoyloxime	0.39
Benzaldehyde O-Methylcarbamoyloxime	0.48
4-Chlorobenzaldahyde O-Methylcarbomoyloxime	0.36
3,4-Dichlorobenzaldehyde O-Methylcarbomoyloxime	0.39
3-Phenoxybenzaldehyde O-Methylcarbomoyloxime	0.29
4-Phenoxyphenylurea	0.69

A striking feature of these values is their similarity. All of the other substituted phenylureas tested had degradation rates too slow to measure over the time scale of the experiments (24-48 hours). The same was true for aldicarb and aldicarb sulfone (aldoxycarb). Menzie (1980) provides an annotated bibliography of papers which may contain quantitative information about the degradation of pesticides in plants. Fletcher et al. (1985) also describes the PHYTOTOX database. This database contains information from over 3500 publications concerning the effects of herbicides on plants and may also contain quantitative information on the degradation of chemicals in plants.

TABLE 6-36. PLANT GROWTH PARAMETERS, CROP SPECIFIC VALUES

	Soybean	Alfafa	Corn	Grain Sorghum	Wheat	Barley	Oats	Sunflower	Cotton	Peanut	Pine
BE	25	20	40	35	47	35	35	25	17.5	20	11.5
FGK	0.31	0.25	0.50	0.50	0.42	0.42	0.42	0.31	0.50	0.42	0.76
TOPT	25	20	25	27.5	15	15	15	25	27.5	25	25
TBASE	10	4	8	10	0	0	0	10	12	13.5	2
LAImx	5	5	5	5	8	8	8	5	5	5	5
FLAI	0.9	0.9	0.8	0.8	0.8	0.8	0.8	0.75	0.85	0.75	0.9
HGTmx	1.5	1.25	2.5	1.5	1.2	1.2	1.2	2.5	1.0	2.0	20
RZ	200	200	200	200	200	200	200	200	200	200	150

6.6.3 KOW--Octanol Water Partition Coefficient

The octanol water partitional coefficient is widely reported for many chemicals, e.g., Rao and Davidson 1980). Either K_{ow} or solubility is required data for the registration of most chemicals and should be readily available. If solubility, and not K_{ow}, is available, relationships in Lyman et al. (1982) can be used to estimate values of the latter. Values selected should be consistent with similar coefficients (K_{oc}, K_d) in other parts of the model.

6.6.4 KP--Partition Coefficient

The partition coefficient used in TEEAM describes the partitioning between the water of the transpiration stream and the nonaqueous organic phases of the aboveground plant biomass. The partition coefficient should be estimated using available data or, alternatively the K_{oc} of the compound and the organic carbon content of the aboveground biomass. K_{oc} may be estimated from solubility (see Section 6.4.1.3) or from K_{ow} (Lyman et al. 1982). The organic carbon content (OC) will vary among plant species and varieties; however, a reasonable approximation of the OC can be made assuming that the makeup of the vascular plant is similar to that of algae use in which the fraction of carbon by weight is approximately 0.36. The partition coefficient is estimated by multiplying the K_{oc} by the organic carbon content (OC).

6.6.5 RHONA--Ratio of Dry Weight to Wet Weight

A reasonable assumption, in the lack of more exact data, is that the living plant is approximately 60 percent water. Assuming a weight of the dry matter of 0.2 g cm^{-3}, then the dry weight to wet weight ratio is about 15 percent.

6.7 APUM MODULE

Guidance for estimating parameters of the APUM module is categorized into three areas:

- Species Abundance
- Animal Movement
- Feeding, Uptake, and Depuration

6.7.1 Species Abundance

TEEAM does not utilize or simulate the number of individuals within the ecosystem; rather, it makes use of the biomass of each species. Biomass of each species remains constant over the period of the simulation in the current version of the model. Estimates must be provided for each species. If it is desirable to obtain a sense of variability of predicted body burden concentrations, etc., in a species caused by differences in movement, feeding, or other characteristics of subgroups of the population, the user may divide the species population into several subgroups. In this case, biomass estimates must be provided for each subgrouping. The user must also differentiate between the biomass of each species present in each habitat of the ecosystem which are not habitat mobile.

The most logical way to specify the biomass of each species is to begin with the end-of-the-foodchain species. Assume that this individual (or pair of individuals) represents the biomass of that species in its territory. Once the territorial area is known, the biomass of the lower trophic-level species can be estimated by multiplying the area (L^2) by an appropriate biomass density for each species of concern ($M\ L^{-2}$). Species of concern could be any of the species which form part of the foodchain for the end-point species. Examples of these organisms in the soil and their prey/predator relationships are shown in Table 6-37.

Densities for some of the more important species are discussed in the following sections.

6.7.1.1 Earthworms--Table 6-38 taken from Lofty (1974) shows biomass estimates for earthworms in soils under a variety of land uses. Biomasses range from 1.6 to 287 g m^{-2}. Higher values are associated with grasslands, while lower values tend to be associated with woodland and arable land.

6.7.1.2 Enchytraeids--White or pot worms are common larger oligochaetes which tend to inhabit the top 3 inches or so of the soil if the humidity is fairly constant. Their numbers undergo wide swings seasonally (Smith 1966). Odum (1971) gives density values of 1-3 g m^{-2} for pasture soils and 7 g m^{-2} for mor-type soils of Denmark.

6.7.1.3 Microarthropods--These consist primarily of mites and springtails. The most numerous are the mites. Odum (1971) indicates biomass of 2 to 5 g m^{-2}. Harding and Studdard (1974) give estimates ranging from 0.03 to 3.2 g m^{-2} for springtails and 0.3 to 5.4 g m^{-2} for mites.

6.7.1.4 Macroarthropods--Macroarthropods include primarily woodlice, millipedes, termites, fly larvae, and beetles. Edwards (1974) gives a biomass density of 2.1 g m^{-2} for woodlice in grassland of a British wood. Edwards (1974) gives population estimates for millipedes ranging from 2.3 to 300 m^{-2}. Using an assumed average weight of 3 mg per individual, this translates to biomass densities of 0.007 to 0.9 g m^{-2}. An average for woodland is probably on the order of 0.3 g m^{-2}. Beetles and fly larvae are estimated to have biomass densities on the order of 1.5 g m^{-2} (Edwards 1974). Termites are estimated to have biomass densities of 5 to 50 g m^{-2}.

6.7.1.5 Molluscs--Mason (1974) gives information on the population biomass of snails living in a beech wood. Twenty-one species were reported, with their total biomass being on the order of 0.7 g m^{-2} dry weight. Estimates ranging from 0.08 to 8.2 g m^{-2}. A reasonable estimate for grasslands appears to be 3 to 7.5 g m^{-2}.

TABLE 6-37. EXAMPLES OF MICROPHYTIC FEEDERS AND OF CARNIVORES WHICH ACT AS SECONDARY AND TERTIARY CONSUMERS WITHIN OR ON TOP OF THE SOIL

Microphytic Feeders		Carnivores			
		Secondary Consumers		Tertiary Consumers	
Organism	Microflora Consumed	Predator	Prey	Predator	Prey
Springtails:	Algae Bacteria Fungi	Mites:	Springtails Nematodes Enchytraeids	Ants:	Spider Centipedes Mites Scorpions
Mites:	Fungi Algae Lichens	Centipedes:	Springtails Nematodes Snails Slugs Aphids Flies	Centipedes:	Spiders Mites Centipedes (other)
Protozoa:	Bacteria and other microflora				
Nematodes:	Bacteria Fungi	Moles:	Earthworm Insects	Beetles:	Spiders Mites Beetles (other)
Termites:	Fungi				

Source: After Brady 1974.
Note: In the current version of TEEAM, soil dwelling organisms may not prey on one another. Degree of uptake is specified through the use of bioconcentration factors.

6.7.2 Animal Movement

Animal movement input data include the frequency of movement, movement transition matrices, and initial or steady state population distributions. Because these data are highly species-specific, it is not possible to provide detailed steps for parameter estimation. However, some general guidance is provided in the following paragraphs regarding the types of data available and the interpretation of these data for TEEAM input.

6.7.2.1 NMOVE--The Frequency of Animal Movement--

This parameter is used in the model to specify how often the animal's location is recomputed within each day. NMOVE will probably depend upon how often the animal feeds during the day. For instance, animals which feed during the early morning and late afternoon might move between their nesting locations and feeding locations four times each day. This parameter could also be limited by the animal's rate of movement and the distance between locations.

6.7.2.2 PMVC--The Soil Horizon Transition Matrix for Soil Animals--
This matrix contains the conditional probabilities that a soil animal will move to each soil horizon given its initial horizon location. It is input only for soil animals which do not move between TEEAM habitats and is not required for animals modeled using a steady-state population distribution. The transition matrix for soil animals will often depend on environmental conditions such as temperature and moisture. For instance, earthworms will generally move deeper into the soil column in response to extreme surface temperatures (Lee 1985). When soil horizons become saturated, earthworms move towards the surface to breathe. Earthworms may also exhibit preferences for certain soil types with high organic matter contents. The transition matrix should be formulated to represent these environmental factors and should also reflect the relative locations of the various soil horizons, their thicknesses, and the travel time of the animal.

6.7.2.3 PMVH--The Habitat Transition Matrix for Higher Animals--
This matrix contains the conditional probabilities that an animal will move to each habitat given its initial habitat location. It is not required for soil animals and for animals modeled using a steady-state population distribution. The habitat movement matrix should reflect both quantitative animal movement data and the user's qualitative understanding of the animal's movement between nesting and feeding habitats. Table 6-39 lists habitat information for mallard ducks in Nebraska, and is an example of the types of data from which habitat transition matrices can be derived. In general, these data indicate that mallard ducks prefer to feed in the grazed corn stubble habitat. However, distances from the nest to the various

TABLE 6-38. POPULATIONS OF EARTHWORMS IN DIFFERENT HABITATS

	Site	No. m^{-2}	gm^{-2}
Arable land	Bardsey Island, U.K.	287	76
Arable land	Herts., U.K.	18	1.6
Arable land with dung	Herts., U.K.	79	39.9
Fallow soil	U.S.S.R.	18.5-33.5	4.6-8.4
Orchard with grass	Cambs., U.K.	848	287
Orchard with grass	Holland	300-500	75-122
Pasture	N. Wales	481-524	112-120
Pasture	Westmorland, U.K.	389-470	52-110
Under pig litter	U.S.A.	960	272
Pseudotsuga mor	N. Wales	14.0	4.7
Mixed woodland	N. Wales	157	40
Quercus woodland	Hants., U.K.	184	68
Pinus woodland	Hants., U.K.	40	17

feeding habitats indicate that the ducks might utilize the nearest habitat at times. Information on the times of day at which these animals feed in each habitat could be used to further refine the transition matrix.

6.7.2.4 PHAB--The Distribution of Animal Populations--

This array contains the fraction of the animal population located in each habitat (or soil horizon for soil animals). It is not required for animals modeled by random subgroup movement. For populations which are not at steady state, PHAB serves as an initial condition for movement calculations and might be used to specify the distribution at the start of a season. For steady-state populations the input distribution remains constant throughout the simulation, and should reflect the long-term average population distribution. For instance, if the locations of mallard ducks were assumed to be constant, the percent use data in Table 6-39 could be used as the population distribution.

6.7.3 Feeding, Uptake, and Depuration

The user must specify feeding and chemical uptake and depuration rates in order to simulate biomagnification in the terrestrial food chain. The specification of these rates is somewhat different for animals living in or on the soil versus higher tropic level animals.

TABLE 6-39. USE OF VARIOUS HABITATS BY MALLARD DUCKS IN NEBRASKA

Habitat	Availability (%)	Percent Use	Distance from Nest (km)
Corn Stubble	16.8	4.6	3
Cultivated Corn Stubble	2.7	2.3	3.1
Plowed Corn Stubble	5.1	1.1	1.8
Grazed Corn Stubble	72.1	75.9	3.8
Feed lot	0.4	16.1	3.6

Source: Jorde et al. 1983.

6.7.3.1 Total Food, Water, and Air Intake Rates--

Food, water, and air intake rates must be specified for each species as appropriate. Soil dwelling organisms do not require input of water or air consumption rates.

Feeding rates have been reported for many of the more common organisms that live in the soil. Shown in Table 6-40 are mean intake rates, range of intake rates, and food assimilation efficiencies. Although assimilation efficiencies are not utilized directly by the model for soil dwelling species, intake rates should be adjusted downward by multiplying the gross intake rates by the assimilation efficiency. It should be recognized that for these organisms, metabolic rates and therefore food intake rates are affected by temperature. Lower soil temperatures are associated with lower food intake rates.

For avians, higher food intake rates, per gram of body weight, are associated with smaller species. Welty (1962) gives food consumption rates for these species:

• European Robin (16 grams)	$14.7\ gg^{-1}\ day^{-1}$
• Song Thrush (89 grams)	$9.8\ gg^{-1}\ day^{-1}$
• Quail (170 grams)	$8.8\ gg^{-1}\ day^{-1}$

Dorst (1974) states that avians weighing between 100 to 1000 g consume 5 to 9% of their body weight per day, while those weighing 10 to 100 g consume from 10 to 30% of their body weight per day. Little information was found in the literature concerning the assimilation efficiency of food items by avians. Farner et al. (1972) give some information on the absorbability of fatty acids in the digestive tract of chickens. These data may be representative of the assimilation efficiency of food items and pesticides in the diet of avians:

Fatty acids	4 - 95%
Monoglycerides	41 - 100%
Triglycerides	76 - 96%
Hydrolyzed Triglycerides	67 - 93%

Welty (1975) also gives information on the water consumption rates of birds. These rates also vary on a function of size with higher utilization rates per body weight also associated with smaller species as follows:

• Wren (12 grams)	$0.37\ gg^{-1}\ day^{-1}$
• Junco (21 grams)	$0.16\ gg^{-1}\ day^{-1}$
• Whippoorwill (40 grams)	$0.07\ gg^{-1}\ day^{-1}$
• Quail (144 grams)	$0.04\ gg^{-1}\ day^{-1}$

Welty (1975) also notes that ground doves that consumed 0.1 $gg^{-1}\ day^{-1}$ of water at normal temperatures, consumed 0.3 gg^{-1}/day^{-1} at temperatures of 30 to 40°C.

Farner et al. (1972) give a regression for the respiration rate (R) of birds in ml min^{-1} as a function of body weight (W) in kg.

TABLE 6-40. FOOD INTAKE RATES AND ASSIMILATION EFFICIENCIES FOR VARIOUS COMMON SOIL DWELLING ORGANISMS

Organism	Intake Rate (gg^{-1} day^{-1})		Assimilation Efficiency (%)	Reference
	Mean	Range		
Earthworms		0.1 to 0.3	1.3-2.8	Lofty 1974; Lee 1985
(Savannah species)		4 to 6		Lee 1985
(European forest lumbricid)	0.1			Lee 1985
Molluscs	0.025	0.01 to 0.04	50 ± 6	
Millipedes	0.01	0.005-0.04	4 - 50	Edwards 1974
Woodlice	0.03		10-70	Edwards 1974
Termites	0.025	0.02 to 0.03	60	Edwards 1974
Diptera and/or Coleoptera (Fly larvae and/or Beetles)	0.3	--	--	Edwards 1974
Orbatids (mites)	0.2	0.06-0.40	14	Harding and Stuttard 1974
Collembola (Springtails)	0.14	0.018-0.046	--	Harding and Stuttard 1974

$$\log R = \log 284 + 0.77 \log W \qquad (6\text{-}19)$$

No information was found concerning the trapping efficiency of pesticides in the avian lung.

6.7.3.2 Food Preferences--

Food preference factors must be established for each species simulated. A generalized food web for soil dwelling species was shown in Table 6-37, based on information found in Brady (1974). For the purposes of this model, the uptake of pesticides by soil-dwelling organisms is based on biocentration factors. Soil-dwelling organisms do not feed on others. In reality, earthworms and millipedes feed on detritus and soil. Snails and slugs will feed on both detrital material at the soil surface and also on living plant matter. Centipedes may feed on snails and slugs and other centipedes. Beetles may feed on mites and other beetles, while ants may feed on centipedes and mites. Avians are allowed to feed on other organisms and might feed on ants, centipedes, beetles, earthworms, snails and slugs, mites, millipedes and plant matter, directly. The user has the perogative as to which species will be simulated and what their food preferences will be.

An abundance of food preference information is available for most common avians. Food preferences may vary widely with season, sex, habitat, and availability of food items. Frequently, for females, consumption of animal material in the diet increases during nesting season. Some general guidance for passerines (esp. T. migratorius), mallard ducks and bobwhite quail is given in the following discussion.

The American robin (T. migratorius) has a diet which consists, on the average, of 60% plant matter and 40% animal matter (Bent 1949). The plant consists chiefly of wild berries and fruits; seeds do not comprise a large portion of the diet. During winter, the diet consists almost exclusively of plant material. Animal materials consist of beetles, caterpillars, hymenoptera, flies, and grasshoppers. According to Bent, an eastern robin's diet was observed to consist of the following:

Food Item	Frequency of Occurrence (%)
Plants:	81.5
Bar berry	61
Sumach	29
Coral berry	4.5
Animals:	93.5
Beetles	82.5
Millipedes	38.5
Ants	27.0
Cutworms	9.5
Sowbugs	6.5
Wireworms	4.0
Flies	3.0
Cockroaches	1.5

Earthworms are also taken from pastures and lawns.

Western robins in Utah between April and July were observed to have the following food preferences:

Food Item	Percentage in Diet
Alfalfa weevil	14
Cutworms	23
Click beetles	11
Earthworms	9
Flies	6
Dung beetles	6
Ground beetles	4

Beetles made up 54% of the diet in April, but only 13% from November to April.

Swanson et al. (1985) give the data on food preferences for mallard ducks shown in Table 6-41. Food preferences of mallards wintering in south central Nebraska (Jorde et al. 1983) were even more dominated by plant matter:

TABLE 6-41. PROPORTION BY VOLUME (%) OF PLANT AND ANIMAL FOODS IN THE ESOPHAGI OF MALLARDS COLLECTED DURING SEASONS OF 1974-80 IN SOUTH CENTRAL NORTH DAKOTA

Food	Male n = 39	Nonlaying Female n = 41	Laying Female n = 37
Total Animal	37.6	37	71.9
Gastropoda	6.3	4.5	16.4
Insects	16.8	22.6	27.1
Coleoptara	0.5	2.5	4.8
Lepidoptera	--	1.5	2.8
Crustacea	11.3	7.5	12.9
Oligochaeta	--	--	11.8
Total Plant	62.4	63	28.1
Seeds	56.4	58.5	24.8
Vegetation	6.0	4.5	3.3
Roots/tubers	4.1	3.9	2.8

Source: Swanson et al. (1985)

Food Item	Percentage by Weight
Plant:	97
Seeds	
Corn	46
Milo	2
Polygonum spp.	11
Vegetation	
Lemna minor	16
Animal:	3
Mollusks	3
Insects	—

In general, information on the habits and feeding preferences of ducks may be found in the following references:

Belrose, F.C. 1976. Ducks, Geese and Swans of North America. Stackpole Books. Harrisburg, PA. 543 pp.

Martin, A.C. and F.M. Uhler. 1939. Food of Game Ducks in the United States and Canada. U.S. Dept. of Interior, Fish and Wildlife Service Research Rpt. No. 30. 308 pp.

McAtee, W.C. 1918. Food Habits of the Mallard Ducks of the United States. U.S. Dept. of Agriculture Bull. 720. 35 pp.

6.7.3.3 Depuration Rates--

Depuration or clearance rates vary widely with chemical and species. While higher clearance rates would appear to be associated with higher metabolic rates and hydrophilic compounds, exceptions appear in the literature. A summary of the clearance rates found in the literature for a wide range of species and compounds is shown in Table 6-42. Wide variation is found for the carbanate insecticides, even within the same species. Clearance rates for the more hydrophobic chlorinated hydrocarbons are, in general, lower, with the exception of clearance rates for dieldrin calculated from data for wood thrushes reported by Jeffries and Davis (1968). The more hydrophobic hexachlorobenzene apparently cleared slugs faster than 2,4-D.

Clearance rates can be calculated for soil dwelling species using the bioconcentration factor concept. The concentration in a soil dwelling species can be modeled using:

$$M_o \frac{dC_o}{dt} = K_t C_t V_t - K_m C_o M_o \qquad (6\text{-}20)$$

in which K_t is the uptake rate from the soil,
C_t is the total soil concentration,
V_t is the volume of soil having concentration, C_t,
K_m is the metabolic clearance rate, and
C_o is the concentration of pesticides in the organism.

or

$$\frac{dC_o}{dt} = \frac{K_t C_t V_t}{M_o} - K_m C_o \qquad (6\text{-}21)$$

assuming that the organism mass M_o does not change over time. At steady state:

$$\frac{K_t C_t M_t}{M_o} = K_m C_o \qquad (6\text{-}22)$$

Rearranging terms:

$$\frac{K_t V_t}{K_m M_o} = \frac{C_o}{C_t} \qquad (6\text{-}23)$$

TABLE 6-42. DEPURATION RATES FOR VARIOUS PESTICIDES IN VARIOUS ANIMAL SPECIES FOUND IN THE LITERATURE

Species	Chemical	K_{ow}	Rate (day^{-1})	References
Earthworm	Aldicarb sulfoxide	5	0.88[a]	Roberts and Dorough (1985)
	Carbofuran	207	0.04[a]	
	Carbofuran	207	0.43[a]	
	Carbofuran and Oxamyl	207	6.9[a]	
L. Terrestris	Carbofuran	207	0.05[a]	
E. Foetida	Carbofuran	207	1.5[a]	
	Dieldrin	4,930	7.3E-4[a]	Lee (1985)
	Heptachlor epoxide	7,370	6.3E-4[a]	
	DDT	50,000	5.9E-4[a]	
Slug	2,4-D	416	0.001[b]	Haque and Ebing (1983)
	Hexachlorobenzene	1,000,000	0.16[b]	
Wood Thrush	Dieldrin	4,930	1.3[b]	Jeffries and Davis (1968)
Herring Gull	Dieldrin	4,930	0.0026[a]	Norstrom et al. (1986)
Grackle	DDE		0.003[a]	Stickel et al. (1984a) (See Section 6.7.3.3)
	Mirex		0.0035[a]	
	Oxychlordane		0.01[a]	
	Arachlor 1254		0.0077[a]	Stickel et al. (1984b) (See Section 6.7.3.3)

[a] Reported in the reference.
[b] Calculated from data in the reference.

Since the bioconcentration factor BCF is defined as the concentration in the organism over that in the soil:

$$\frac{K_t V_t}{K_m M_o} = BCF \qquad (6\text{-}24)$$

Furthermore, the term V_t/M_o can be written as $\Delta z/\rho_o$ where Δz is the depth of soil having concentration C_t (m) and ρ_o is the organism density (gm^{-2}), so that 6-24 can be rewritten as:

$$\frac{K_t \Delta z}{K_m \rho_o} = BCF \qquad (6\text{-}25)$$

Using 6-25, and knowing the intake rate, the metabolic clearance rate, K_m, can be chosen to yield field observed bioconcentration factors. Bioconcentration factors for a variety of pesticides in earthworms range from less than 1 to 10 with the norm being about 5. Bioconcentration factors for slugs are somewhat higher ranging from 1 to 100 (Thompson and Edwards, 1974). The data of van Gestel and Ma (1987) give a range of bioconcentration factors for various chlorinated phenols in earthworms of 0.4 to 5.3. No bioconcentration factors were found in the literature for other soil animals.

Some specific references on accumulation and clearance rates for avians appear below. Not all of these references have been reviewed by the authors of this report.

Bailey, S., P.J. Bunyan, B.D. Rennison and A. Taylor. 1969. The Metabolism of 1,1-di (chlorophenyl)-2,2-di-chloroethylene and 1,1-di(p-chlorophenyl)-2-chloroethylene in the Pigeon. Toxicol. Appl. Pharmacol. 14:23.

Baldwin, M.D., J.W. Crawford, D.H. Hutson and D.L. Street. 1976. The Metabolism and Residues of (^{14}C) Endrin in Lactating Cows and Laying Hens. Pesticide Sci. 7:575-594.

Charnetski, W.A. 1976. Organochlorine Insecticide Residues in Ducklings and Their Dilution by Growth. Bull. Environ. Contam. Toxicol. 16:138-144.

Cummings, J.G., M. Eidelman, V. Turner, D. Reed, K.T. Zee and R.E. Cook. 1967. Residues in Poultry Tissues from Low Level Feeding of Five Chlorinated Hydrocarbon Insecticides to Hens. J. Assoc. Off. Anal. Chem. 50:418-425.

De Vos, R.H., J. Bruman and A.B. Engel. 1972. Residues of Organochlorine Pesticides in Broilers from Feed Fortified with Known Levels of These Compounds. Pesticide Sci. 3:421-432.

Fries, G.F., R.J. Lillie, H.C. Cecil and J. Bitman. 1977. Retention and Excretion of Polychlorinated Biphenyl Residues by Laying Hens. Poultry Sci. 56:1275.

Haseltine, S.D., M.T. Finley and E. Cromartic. 1980. Reproduction and Residue Accumulation in Black Ducks Fed Toxaphene. Arch. Environ. Contam. Toxicol. 9:461-471.

Heinz, G.H. and R.W. Johnson. 1979. Elimination of Endrin by Mallard Ducks. Toxicology. 12:189-196.

Hicks, B.W., H.W. Dorough and R.B. Davis. 1970. Fate of Carboforan in Laying Hens. J. Econ. Entomol. 63:1108-1111.

Kan, C.A. and J.C. Jonker-Den Rooyen. 1978. Accumulation and Depletion of Some Organochlorine Pesticides in High-Producing Laying Hens. J. Agric. Food Chem. 26:935-940.

Stadelman, W.J., B.J. Liska, B.E. Langlois, G.C. Mostert and A.R. Stemp. 1965. Persistence of Chlorinated Hydrocarbon Insecticide Residues in Chicken Tissues and Eggs. Poultry Sci. 44:435-437.

Stikel, L.F., W.H. Stikel, R.D. McArthur and D.L. Hughes. 1979. Chlordane in Birds: A Study of Lethal Residues and Loss Rates. In: Toxicology and Occupational Medicine. W.B. Deichman (organizer). p. 387-396. Elslevier/North Holland, N.Y.

Stikel, W.H., J.A. Galyen, R.A. Dyrland and D.L. Hughes. 1973. Toxicity and Persistence of Mirex in Birds. In: W.B. Deichman (ed.) Pesticides and the Environment: A Continuing Controversy. p. 437. Intercontinental Medical Book Corp., NY.

Stikel, W.H., L.F. Stikel, R.A. Dyrland and D.L. Hughes. 1984a. DDE in Birds: Lethal Residues and Loss Rates. Arch. Environ. Contam. Toxicol. 13:1-6.

Stikel, W.H., L.F. Stikel, R.A. Dyrland, and D.L. Hughes. 1984b. Arochlor 1254 Residues in Birds: Lethal Levels and Loss Rates. Arch. Environ. Contam. Toxicol. 13:7-13.

6.7.3.4 LD50, LD10 - Lethal Dosages--

Little information was retrieved for lethal dosages for either soil dwelling organisms or avians. Lee (1985) provides an extensive table of LD values of various chemicals to earthworms. Unfortunately, the units given are kg a.i. ha^{-1} and are incompatible with the units required by TEEAM. The information necessary to compute an LD50 based on dosage per gram of the predator are not available in Lee. However, the reference given for the data, Ruppell and Laughlin (1976), may contain more information. Lee does give some LD50 information for some fungicides (benomyl, carbendagin, thiabendazole). The LD50 for these chemicals is reported as 10 μg/worm. Given an individual biomass of about 1 gram, the LD50 would be 10 μg g^{-1} or 10^{-5} μg mg^{-1}. The original reference for this data is Wright (1977).

The LD50, LD10 parameters are important to the operation of the TEEAM code in order to produce reasonable body burden concentrations in upper trophic level species. The population of the species is not modeled, and therefore mortality due to pesticide accumulation of individals of the species cannot be accounted for. Because of this limitation, the species will accumulate pesticides, based on the difference between intake and depuration rates, approaching a quasi-equilibrium level. This level may be much greater than normally would be observed because lethal effects would eventually limit the intake. Therefore, the LD values are used to adjust the intake rates so that unreasonable values of body burden concentrations are not simulated. In lower trophic level species (i.e., soil dwelling animals) this is not a problem because the depuration rates would normally be calculated from the bioconcentration factor (BCF). Therefore, the correction is not applied to soil dwelling animals.

Lee (1985) also reports on the work on Hill et al. (1975) who determined lethal dietary concentrations to bobwhite quail, Japanese quail, ring-necked pheasants and Mallard ducks to be 311 to 1869 μg g^{-1} for DDT, 37 to 169 μg g^{-1} for dieldrin and 92-480 μg g^{-1} for heptachlor. Barker (1958) reported poisoning of robins to be associated with dietary concentrations of 53-204 ug g^{-1}. Collett and Harrison (1968) found that levels of DDT taken as food by blackbirds and thrushes were 13 to 29 μg g^{-1}. Again, the units of these LC50s are incompatible with the LD50 required by the model. The model LD50 is the 50 percent mortality lethal dosage for unit weight of the bird. Information required to convert to these units (i.e., the food intake and weight of the birds) is not available in Lee but may be available in the original references.

6.8 SENSITIVITY OF TEEAM TO INPUT PARAMETER VALUES

A sensitivity analysis was performed on TEEAM to determine which input parameters have the strongest effect on model outputs. The results of this analysis give insight into the effects of uncertainty and should provide some guidance to the user on where to concentrate data collection efforts. The methodology and results used in the TEEAM sensitivity analysis are summarized in the following paragraphs.

6.8.1 Sensitivity Analysis Approach

The base data set for this sensitivity analysis is the peanut field ecosystem discussed in Section 8. The target species is the American Robin. These birds are exposed to pesticides, in this example, through ingestion of soil and water, inhalation of vapors, and predation on earthworms. The base simulation has a duration of thirty days, with pesticide applied to soil on the first day of simulation.

The sensitivity of this system to input parameters was evaluated by running TEEAM in its Monte Carlo mode for 500 runs. Probability distributions for input parameters were assumed based on best estimates of their range of uncertainty; Table 6-43 lists the various input parameters and their assumed probability distributions. The analysis was performed for two cases: 1) uncorrelated inputs and 2) correlated inputs. For case 2, correlations were initially assigned as high (.7), medium (.5), or low (.2), and then adjusted by trial and error until a positive-definite correlation matrix was found. The correlation matrix is shown in Figure 6.8. Two output parameters were evaluated: 1) maximum 5-day average dosage to the target species and 2) maximum 5-day average concentration of pesticide in the target species.

The TEEAM Monte Carlo simulation of the robin-peanut field ecosystem provided 500 independent realizations of dosage and concentration output derived from randomly selected input data. Sensitivity of these model outputs was then evaluated by stepwise regression analysis. In stepwise regression, the importance of each input variable is evaluated by comparing the sum of squares due to the regression to the sum of squares due to residual errors, as quantified by an F-statistic. In the first step, the input variable with the highest correlation coefficient is added to the regression model and tested for significance. Other variables are brought into the regression and tested for significance until no more variables can be added to the regression model. This results in a subset of input variables which contribute significantly (at a specified confidence level) to the regression equation which best estimates model outputs. A 95% confidence level was used for all F-statistic significance tests of TEEAM variables.

6.8.2 Sensitivity Analysis Results

Table 6-44 lists the variables which were most significant in determining pesticide dosage to the target species. Also listed are the individual correlation coefficients. These variables collectively explain 96% of the variance in pesticide dosage. The three most important variables in this case were the pesticide application rate, the bioconcentration factor for earthworms, and the total daily feeding rate for the robins.

Table 6-43. INPUT PARAMETERS USED IN SENSITIVITY ANALYSES AND THEIR ASSUMED DISTRIBUTIONAL PROPERTIES

Parameter	Units	Distribution	Mean	Coefficient of Variation
Soil Bulk Density	g cm^{-3}	Normal	1.45	0.10
Adsorption Partition Coefficient	cm^3 g^{-1}	Log Normal	30.0	1.20
Wilting Point Water Content	cm^3 cm^{-3}	Normal	0.10	0.25
Field Capacity Water Content	cm^3 cm^{-3}	Normal	0.20	0.15
Soil Hydraulic Conductivity	cm hr^{-1}	Log Normal	4.40	1.25
Decay Rate in Soil	$days^{-1}$	Log Normal	0.02	1.00
Decay Rate on Foliage	$days^{-1}$	Log Normal	0.02	1.00
Henry's Law Constant	cm^3 cm^{-3}	Normal	5.8E-5	0.29
Pesticide Application Rate	kg ha^{-1}	Normal	7.50	0.27
Root Reflection Coefficient	Dimensionless	Normal	0.50	0.20
Decay Rate in Plants	$days^{-1}$	Log Normal	0.02	1.00
Octanol Water Partition Coefficient	cm^3 g^{-1}	Log Normal	1052	0.80
Runoff Curve Number	Dimensionless	Normal	78.0	0.05
Bioconcentration Factor for Earthworms	Dimensionless	Normal	7.14	0.20
Metabolic Degradation Rate in Target Species	$days^{-1}$	Log Normal	1.20	1.00
Total Feeding Rate	g g^{-1} day^{-1}	Normal	0.10	0.10
Soil Preference Factor	g g^{-1}	Normal	0.05	0.10
Pond Water Ingestion Rate	l mg^{-1} day^{-1}	Normal	5E-7	0.10
Air Inhalation Rate	l mg^{-1} day^{-1}	Normal	0.0043	0.10

These variables would be expected to have a strong linear effect on dosage since they determine the mass of pesticide available and the mass of pesticide taken up into the foodchain. Other parameters such as soil bulk density, partition coefficients, and pesticide decay rates determine the persistence of the pesticide in soil. Note that in this case the principal exposure routes for the target species were through soil ingestion and predation on earthworms. Correlations between input parameters had little

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	SOIL BUL	PARTITIO	WILTING	FIELD CA	HYDRAULI	PEST DEC	FOLIAR D	HENRYS C	APPLICAT	SOIL/ROO	PLANT/PE	OCTANOL/	CROP CH	BCF	METABOLI	TOTAL FE	SOIL PRE	POND DRI	AIR INHA
SOIL BULK DENSITY	1.0000	-0.3000	-0.3000	-0.3000	-0.3000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PARTITION COEF/SOIL	-0.3000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.5000	0.0000	0.5000	0.0000	0.7000	0.0000	0.3000	0.0000	0.0000	0.0000	0.0000	0.0000
WILTING POINT	-0.3000	0.0000	1.0000	0.7000	0.5000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
FIELD CAPACITY	-0.3000	0.0000	0.7000	1.0000	0.5000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HYDRAULIC COND.	-0.3000	0.0000	0.5000	0.5000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PEST DECAY RATE	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.7000	0.0000	0.0000	0.0000	0.5000	0.0000	0.0000	0.0000	0.5000	0.0000	0.0000	0.0000	0.0000
FOLIAR DECAY RATE	0.0000	0.0000	0.0000	0.0000	0.0000	0.7000	1.0000	0.0000	0.0000	0.0000	0.5000	0.0000	0.0000	0.0000	0.3000	0.0000	0.0000	0.0000	0.0000
HENRYS CONSTANT	0.0000	-0.5000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	-0.2500	0.0000	-0.5000	0.0000	-0.2500	0.0000	0.0000	0.0000	0.0000	0.0000
APPLICATION RATE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SOIL/ROOT REFL COEF	0.0000	0.5000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2500	0.0000	1.0000	0.0000	0.5000	0.0000	0.2500	0.0000	0.0000	0.0000	0.0000	0.0000
PLANT/PEST DECAY	0.0000	0.0000	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.3000	0.0000	0.0000	0.0000	0.0000
OCTANOL/WATER-PART	0.0000	0.7000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.5000	0.0000	0.5000	0.0000	1.0000	0.0000	0.2500	0.0000	0.0000	0.0000	0.0000	0.0000
CROP CH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BCF	0.0000	0.3000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2500	0.0000	0.2500	0.0000	0.2500	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
METABOLIC DEGRAD	0.0000	0.0000	0.0000	0.0000	0.0000	0.5000	0.3000	0.0000	0.0000	0.0000	0.3000	0.0000	0.0000	0.0000	1.0000	0.5000	0.0000	0.5000	0.5000
TOTAL FEEDING RATE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5000	1.0000	0.0000	0.5000	0.5000
SOIL PREFERENCE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
POND DRINKING RATE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000	1.0000	0.5000
AIR INHALATION RATE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000	0.5000	1.0000

Figure 6.8. Correlation matrix used in the sensitivity analyses

Table 6-44. SIGNIFICANT PARAMETERS CONTROLLING PESTICIDE DOSAGE TO THE TARGET SPECIES

Parameter	Correlation Coefficient
Pesticide Application Rate	0.76
Bioconcentration Factor for Earthworms	0.36
Total Feeding Rate	0.36
Soil Bulk Density	-0.22
Pesticide Decay Rate in Soil	-0.20
Soil Preference Factor	0.10
Adsorption Partition Coefficient	0.08

effect on model sensitivity, since the list of significant parameters was identical for both the correlated and uncorrelated cases.

Table 6-45 lists the variables which were most significant in determining pesticide concentration in the target species. As would be

Table 6-45. SIGNIFICANT PARAMETERS CONTROLLING PESTICIDE CONCENTRATIONS IN THE TARGET SPECIES

Parameter	Correlation Coefficient
Metabolic Degradation Rate	-0.52
Pesticide Application Rate	0.24
Bioconcentration Factor for Earthworms	0.15
Total Feeding Rate	0.18
Pesticide Decay Rate in Soil	-0.09
Soil Bulk Density	-0.06

expected, many of the same parameters which contribute to dosage also contribute strongly to concentration. However, in this case the metabolic degradation rate was the most important parameter, indicating that most of the ingested pesticide was broken down and decayed by metabolic processes.

In this simple ecosystem, a few variables were observed to control the output of the model. In an actual ecosystem, it is likely that the dosage to, or concentration in, the species of interest would be controlled by a larger set of factors. However, the results of this analysis do appear to be rational. For instance, the most important factors controlling these outputs are those which affect the major pathways of exposure; in this case, direct ingestion of contaminated soil and soil fauna. Obviously, pesticide application rate, bioconcentration factors, feeding rates, soil ingestion rates, decay rates in soil, and adsorption partition coefficients are the principal parameters controlling these exposure pathways. Therefore, the model user should speculate on the major pathways of exposure, and concentrate parameter estimation efforts on those which most directly control concentrations in important media and the uptake of pesticide from these media to the species of interest.

SECTION 7

MODEL OUTPUT

7.1 INTRODUCTION

Each TEEAM module produces some form of output. In general, this output consists of echoed input, tabular event-based or periodic summaries of ecosystem status, or time series files which are Lotus compatible and can be exported for plotting. The following sections describe the output which is or may be produced from each module.

7.2 INPREA

The INPREA module produces output which echoes the input provided by the user in a readable format. The input contained in the files having the following logical unit numbers:

- KRUN (Simulation control)
- KPGDEF (Plant growth parameters)
- KPZDEF (TFAT parameters)
- KMCIN (Monte Carlo parameters)
- KADIN (Animal model parameters)
- GRDEF (grid/habitat map and spray application control parameters)

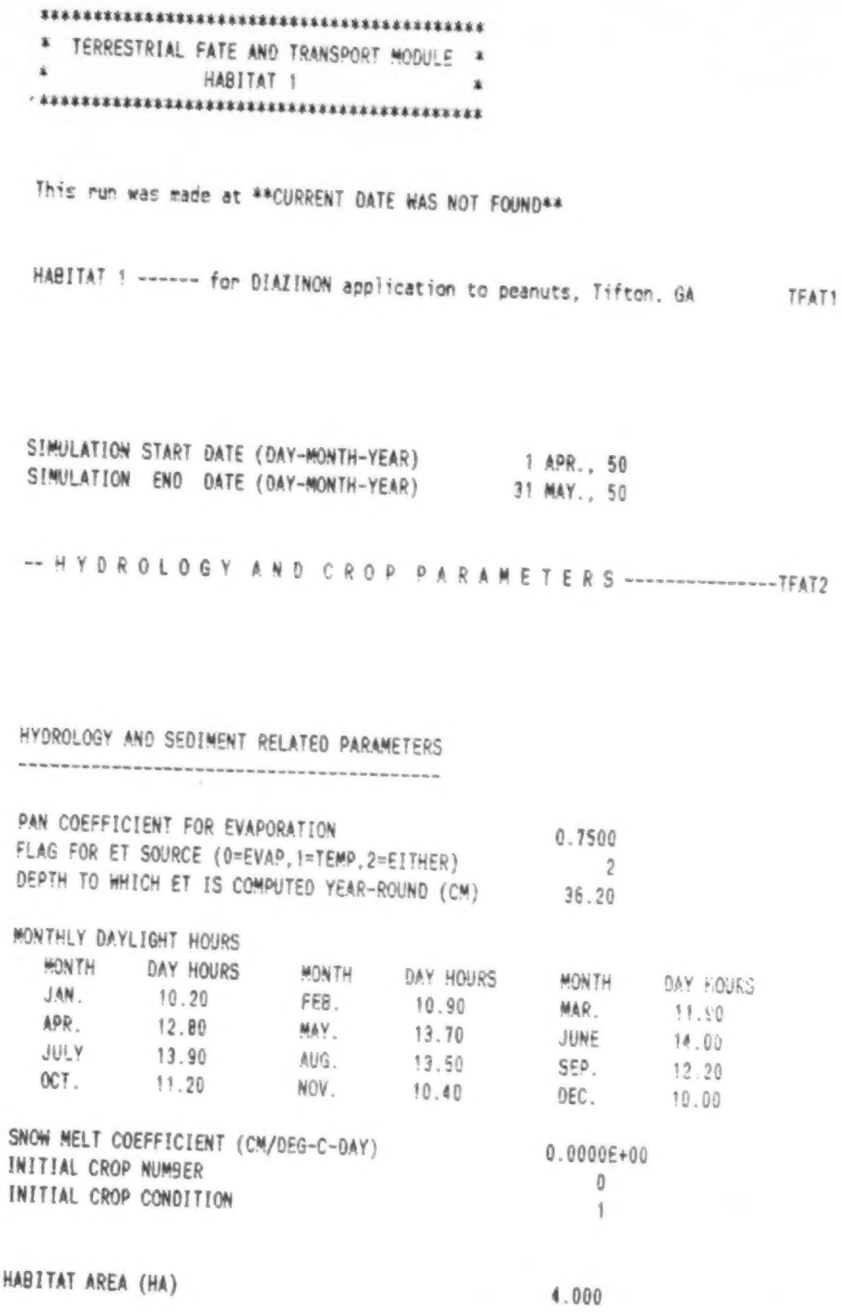
is output to the single KECHO file. An example of the echoed input of each of these files is shown in Figures 7.1 through 7.4.

7.3 FSCBG

The FSCBG model produces an output to a scratch file each time the model is called from within the daily loop of the execution supervisor (EXESUP). It produces an output of the type shown in Figure 7.5. This output echoes new input conditions as well as providing a tabular output of the pesticides deposition values at each receptor grid point. Output from each spray application event is stacked sequentially in the output file.

7.4 TFAT

The TFAT module potentially produces four output files. These files contain the following:



```
********************************************
*  TERRESTRIAL FATE AND TRANSPORT MODULE   *
*               HABITAT 1                  *
********************************************


This run was made at **CURRENT DATE WAS NOT FOUND**


HABITAT 1 ------ for DIAZINON application to peanuts, Tifton, GA        TFAT1




SIMULATION START DATE (DAY-MONTH-YEAR)          1 APR., 50
SIMULATION  END  DATE (DAY-MONTH-YEAR)         31 MAY., 50


-- HYDROLOGY AND CROP PARAMETERS ---------------TFAT2



HYDROLOGY AND SEDIMENT RELATED PARAMETERS
-----------------------------------------

PAN COEFFICIENT FOR EVAPORATION                      0.7500
FLAG FOR ET SOURCE (0=EVAP,1=TEMP,2=EITHER)               2
DEPTH TO WHICH ET IS COMPUTED YEAR-ROUND (CM)         36.20

MONTHLY DAYLIGHT HOURS
   MONTH     DAY HOURS     MONTH     DAY HOURS     MONTH     DAY HOURS
   JAN.        10.20       FEB.        10.90       MAR.        11.90
   APR.        12.80       MAY.        13.70       JUNE        14.00
   JULY        13.90       AUG.        13.50       SEP.        12.20
   OCT.        11.20       NOV.        10.40       DEC.        10.00

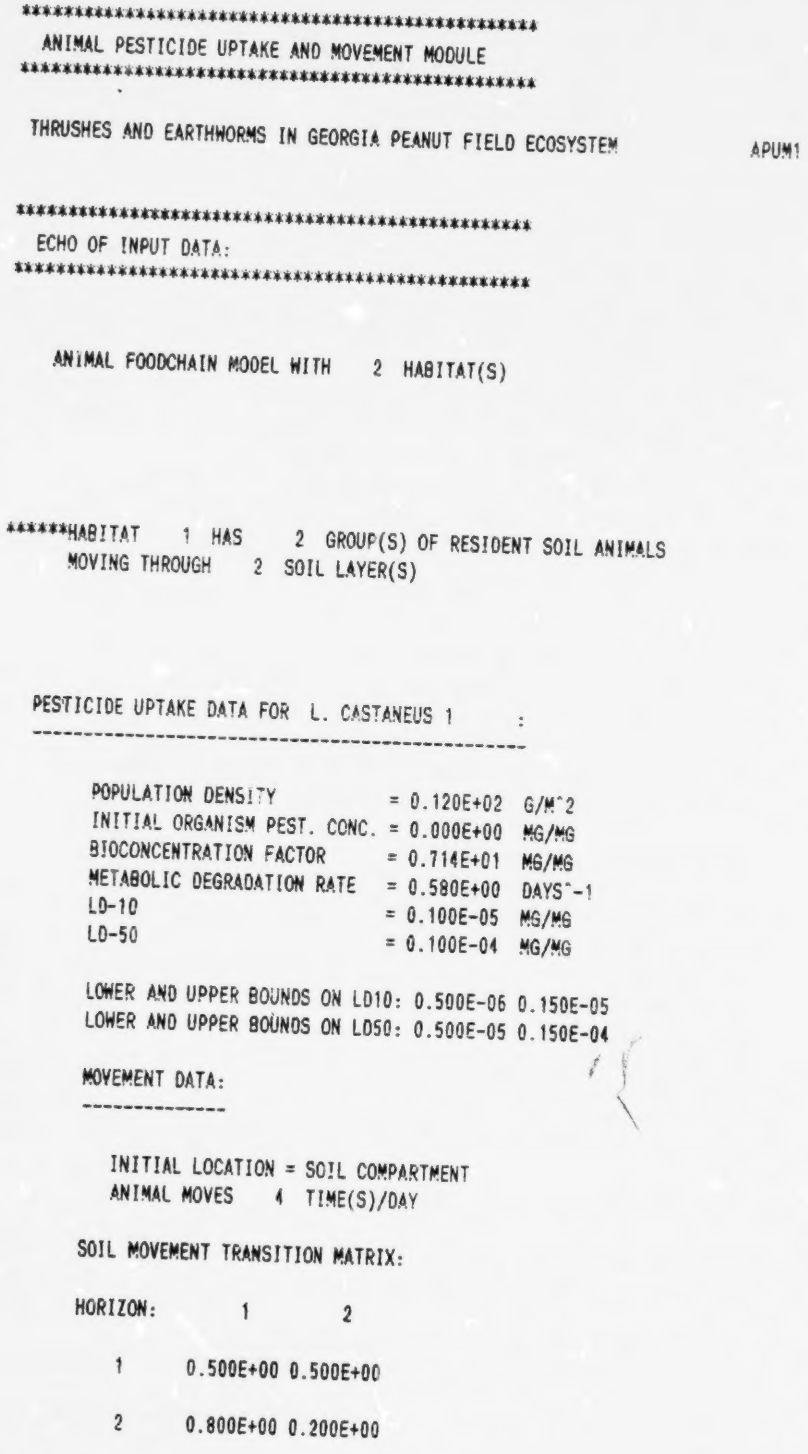
SNOW MELT COEFFICIENT (CM/DEG-C-DAY)               0.0000E+00
INITIAL CROP NUMBER                                        0
INITIAL CROP CONDITION                                     1


HABITAT AREA (HA)                                      4.000
```

Figure 7.1. Example of a portion of the TFAT input echo.

```
1*********************************************************************************
 *              Plant growth and translocation module, habitat  1               *
 *********************************************************************************
 *  Plant number  1
 *
 *  Plant growth parameters:
 *
 * Heat units for plant to mature (C day).................................0.210E+04
 * Rate of conversion of radiation to biomass.................................20.0
 * Maximum leaf area index.....................................................5.00
 * Fraction of season for decline of LAI......................................0.750
 * Ratio of total biomass to crop yield.......................................0.420
 * Maximum root depth (m)......................................................60.0
 * Minimum growth temperature (C)..............................................13.5
 * Optimum growth temperature (C)..............................................25.0
 * Plant height growth coefficient (1/day).....................................1.00
 * Maximum canopy height (m)..................................................0.900
 *
 *  Plant translocation parameters:
 *
 * Reflection coefficient for transfer from the soil to the root (dec.)......1.00
 * First order decay rate (1/day).........................................0.000E+00
 * Octan-1-ol/water partition coefficient.................................0.105E+04
 * Aboveground biomass water content (g/g)....................................0.850
 * Concentration in nonaqueous /concentration in aqueous (cm**3/g)...........315.
 * Ratio of the nonaqueous to the total aboveground biomass (g/g)...........0.150
 *
 *  Plant growth initial conditions:
 *
 * Potential biomass (kg/ha)..............................................0.100E-02
 * Yield (kg/ha)..........................................................0.100E-02
 * Root biomass (kg/ha)...................................................0.100E-02
 * Roots sloughed (kg/ha).................................................0.100E-02
 * Live roots (kg/ha).....................................................0.100E-02
 * Root depth (cm)........................................................0.100E-02
 * Actual biomass (kg/ha).................................................0.100E-02
 * Plant height (m).......................................................0.100E-01
 * Accumulated thermal time...............................................0.000E+00
 *
 *  Plant translocation initial conditions:
 *
 * Concentration in roots (g/g)...........................................0.000E+00
 * Concentration in aboveground biomass (g/g).............................0.000E+00
 *
 *  End of plant growth and translocation data
 *********************************************************************************
```

Figure 7.2. Example of the PLTGRN/PLTRNS input echo.



```
**************************************************
  ANIMAL PESTICIDE UPTAKE AND MOVEMENT MODULE
**************************************************

 THRUSHES AND EARTHWORMS IN GEORGIA PEANUT FIELD ECOSYSTEM            APUM1


**************************************************
  ECHO OF INPUT DATA:
**************************************************


    ANIMAL FOODCHAIN MODEL WITH    2  HABITAT(S)




******HABITAT    1  HAS     2  GROUP(S) OF RESIDENT SOIL ANIMALS
      MOVING THROUGH    2  SOIL LAYER(S)



  PESTICIDE UPTAKE DATA FOR  L. CASTANEUS 1       :
  ------------------------------------------------


       POPULATION DENSITY            = 0.120E+02  G/M^2
       INITIAL ORGANISM PEST. CONC. = 0.000E+00  MG/MG
       BIOCONCENTRATION FACTOR      = 0.714E+01  MG/MG
       METABOLIC DEGRADATION RATE   = 0.580E+00  DAYS^-1
       LD-10                        = 0.100E-05  MG/MG
       LD-50                        = 0.100E-04  MG/MG

       LOWER AND UPPER BOUNDS ON LD10: 0.500E-06 0.150E-05
       LOWER AND UPPER BOUNDS ON LD50: 0.500E-05 0.150E-04

       MOVEMENT DATA:
       -------------


         INITIAL LOCATION = SOIL COMPARTMENT
         ANIMAL MOVES    4  TIME(S)/DAY

       SOIL MOVEMENT TRANSITION MATRIX:

       HORIZON:       1         2

          1      0.500E+00 0.500E+00

          2      0.800E+00 0.200E+00
```

Figure 7.3. Example of a portion of the APUM input echo.

```
     **************************************************
          AERIAL SPRAY TRANSLATION MODULE
     **************************************************


     LOCATION OF HABITATS WITHIN SPRAY MODEL RECEPTOR GRID


     HABITAT COORDINATES
     -------------------


     HABITAT      SOUTHWEST CORNER    NORTHEAST CORNER
                  ----------------    ----------------
        NO.          X         Y         X        Y
                 (METERS)  (METERS)  (METERS) (METERS)
     ------------------------------------------------


         1          0.        0.      140.    280.
         2        140.        0.      280.    280.


     NUMBER OF X-AXIS VALUES IN RECEPTOR GRID =  14
     NUMBER OF Y-AXIS VALUES IN RECEPTOR GRID =  14


                         RECEPTOR GRID AND HABITAT LOCATIONS
                         -----------------------------------


    Y (METERS)

      260.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
      240.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
      220.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
      200.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
      180.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
      160.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
      140.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
      120.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
      100.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
       80.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
       60.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
       40.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
       20.   1 1 1 1 1 1 1 2 2 2 2 2 2 2
        0.   1 1 1 1 1 1 1 2 2 2 2 2 2 2

             0  40  80 120 160 200 240
              20  60 100 140 180 220 260

                      X (METERS)
```

Figure 7.4. Example of a portion of the GRDDEF input echo.

```
1FOREST SPRAY MODEL *** TEEAM/FSCBG: Test 2, Diazinon app. (1 gal/acre), wind dir =270,no evaporation

      *** INPUTS USED BY ALL MODELS ***
  PROGRAM OPTIONS: ISW( 1) =  1
                   ISW( 2) =  0
                   ISW( 5) =  0
                   ISW( 6) =  0
                   ISW(18) =  0
                   ISW(19) =  0
                   ISW(21) =  0
                   ISW(22) =  0
 IS LIQUID WATER OR NON-WATER, 2=NON-WATER, 1=WATER, (IFWATR) = 1
 AIRCRAFT WING SPAN (WNGSPN (METERS)) =  12.60
 HEIGHT OF AIRCRAFT (HGTCFT (METERS)) =   4.00
 DENSITY OF SPRAY LIQUID (DENLIQ (G/CM**3)) =   1.0000
 MOLECULAR WEIGHT OF AIR (AIRMOL) = 28.9600
 BAROMETRIC PRESSURE (AIRPRS (MB)) =1000.00
 RELATIVE HUMIDITY ABOVE THE CANOPY (RELHMO (%)) = 92.000

      *** INPUTS USED BY THE WAKE SETTLING VELOCITY MODEL ***

 AIRCRAFT WEIGHT (ARCRWT (KG)) = 3190.000
 AIRCRAFT GROUND SPEED (ARCRSP (M/S)) =  57.200

      *** INPUTS USED BY THE EVAPORATION MODEL ***

 UPPER LIMITS OF DROP DIAMETERS (DRPUPR (MICRO-M)) =
  611.000, 578.000, 545.000, 512.000, 479.000, 447.000, 414.000,
  382.000, 351.000, 318.000, 284.000, 252.000, 219.000, 187.000,
  154.000, 122.000,  89.000,  56.000,
 LOWER LIMITS OF DROP DIAMETERS (DRPLWR (MICRO-M)) =
  579.000, 546.000, 513.000, 480.000, 448.000, 415.000, 383.000,
  352.000, 319.000, 285.000, 253.000, 220.000, 188.000, 155.000,
  123.000,  90.000,  57.000,  30.000,

      *** INPUTS USED BY THE DISPERSION MODELS ***

 NUMBER OF LINE SOURCES (NSOURC) =   7
 DISTANCE BETWEEN SPRAY LINES (SWATH (M)) =   20.000
 EMISSION OF SPRAY MATERIAL FOR EACH SOURCE (Q (GAL/ACRE)) =
  1.00000E+00, 1.00000E+00, 1.00000E+00, 1.00000E+00, 1.00000E+00,
  1.00000E+00, 1.00000E+00,
 TIME TO SPRAY CLOUD STABILIZATION (TAU (SEC)) =   2.500
 STAND. DEV. OF SPRAY MATERIAL ALONG SPRAY LINE (SIGXYZ (M)) =   2.977
 DECAY COEFFICIENT (DECAY (/SEC)) = 0.00000E-01
 DEPTH OF GAS SOURCES (DELTAH (M)) =   1.000
 LAT., VERT. REFERENCE DISTANCE (XLRZ (M)) =*********
 SURFACE MIXING LAYER HEIGHT (HM (M)) =  200.000
 WIND DIRECTION (FROM) (THETA (DEG)) = 270.00
 RATIO OF LAGRANGIAN TO EULERIAN TIME SCALES (BETA1) = 0.00
 WIND-SPEED SHEAR (DELU (M/S)) = 0.0000
```

Figure 7.5a. Example of the FSCBG input echo.

```
*****************************************************************
FSCBG aerial spray  5/ 5/50
*****************************************************************

    Air temperature (C) =  25.60
    Wind speed (m/sec)  =   3.58
    CALCULATION HEIGHT FOR GRID POINTS (Z (METERS)) =   0.08
    STANDARD DEV. OF WIND DIRECTION ANGLE (SIGAP (RAD)) =0.17453
    STANDARD DEV. OF WIND ELEVATION ANGLE (SIGEP (RAD)) =0.10472
*****************************************************************
       *** FOREST SPRAY MODEL *** TEEAM/FSCBG: Test 2, Diazinon app. (1 gal/acre), wind dir =270,no evaporation
                                                      TABLE  1

                              *-* DEPOSITION    (MICROGRAMS     /SQUARE  METER  ) *-*
                              *-*         AT A HEIGHT OF   0.0815 METERS         *-*
                        (MAXIMUM DEPOSITION    = 9.118761E+05 AT X=   140.000, Y=    60.000, Z=   0.1)

 Y AXIS                                   - X AXIS (METERS) -
(METERS)      0.00        20.00        40.00        60.00        80.00        100.00       120.00       140.00       160.00
                                      - DEPOSITION    -
------------------------------------------------------------------------------------------------------------------------
   260.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72283E+05  8.91148E+05  9.01286E+05  9.07490E+05  9.11620E+05  2.31885E+05
   240.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32253E+05
   220.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
   200.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
   180.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
   160.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
   140.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
   120.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
   100.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
    80.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
    60.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32254E+05
    40.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72289E+05  8.91177E+05  9.01365E+05  9.07646E+05  9.11876E+05  2.32253E+05
    20.00  0.00000E-01  6.82653E+05  8.28733E+05  8.72283E+05  8.91148E+05  9.01286E+05  9.07490E+05  9.11620E+05  2.31885E+05
     0.00  0.00000E-01  3.41326E+05  4.14367E+05  4.36144E+05  4.45589E+05  4.50682E+05  4.53823E+05  4.55938E+05  1.16127E+05

 Y AXIS                                   - X AXIS (METERS) -
(METERS)     180.00       200.00       220.00       240.00       260.00
                                      - DEPOSITION    -
------------------------------------------------------------------------------------------------------------------------
   260.00  8.79570E+04  4.60485E+04  2.84701E+04  1.93634E+04  1.40014E+04
   240.00  8.84450E+04  4.66520E+04  2.91689E+04  2.01250E+04  1.47915E+04
   220.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01412E+04  1.48166E+04
   200.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01414E+04  1.48170E+04
   180.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01414E+04  1.48170E+04
   160.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01414E+04  1.48170E+04
   140.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01414E+04  1.48170E+04
   120.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01414E+04  1.48170E+04
   100.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01414E+04  1.48170E+04
    80.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01414E+04  1.48170E+04
    60.00  8.84471E+04  4.66569E+04  2.91785E+04  2.01412E+04  1.48166E+04
    40.00  8.84450E+04  4.66520E+04  2.91689E+04  2.01250E+04  1.47915E+04
    20.00  8.79570E+04  4.60485E+04  2.84701E+04  1.93634E+04  1.40014E+04
     0.00  4.42236E+04  2.33285E+04  1.45893E+04  1.00707E+04  7.40848E+03
```

Figure 7.5b. Example of the FSCBG output.

- Daily, monthly, or annual habitat hydrology output summaries
- Daily, monthly, or annual habitat pesticide flux summaries
- End of day, end of month, or end of year concentration profiles for each habitat
- Daily time series output (fluxes, concentrations, masses, etc.) for plotting

Examples of the TFAT output files are shown in Figures 7.6 through 7.9. The output is largely self-explanatory. The labels above each column in the time series output file echo the PLOTFL designation for the plotted value.

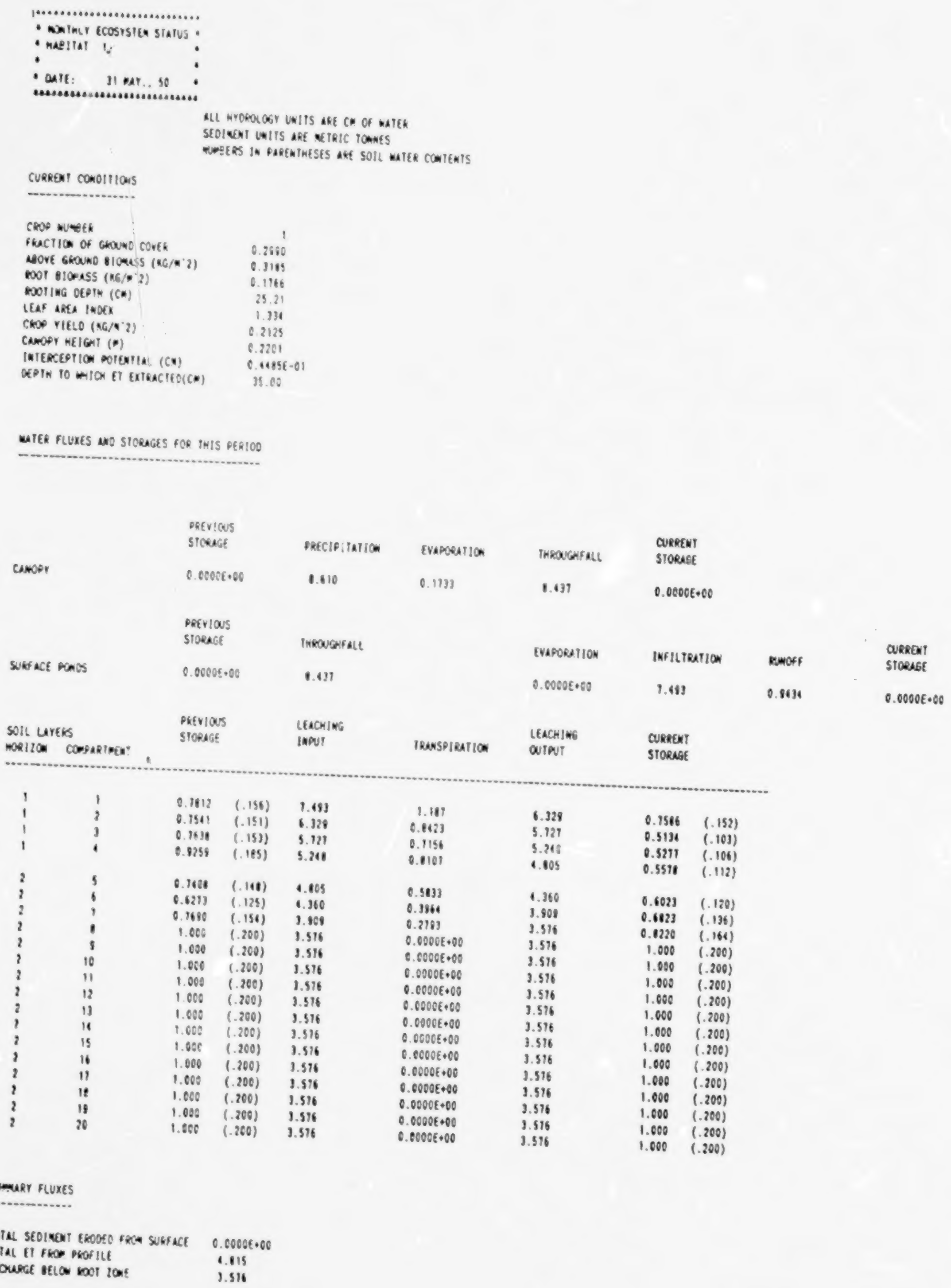
7.5 APUM

The Terrestrial Animal Exposure Model produces two output files. The first output file provides a detailed breakdown of dosages for each simulated animal group, and may be written out daily, monthly, or annually depending on user-selected options. The dosage breakdown for each animal, illustrated in Figure 7.10, includes total cumulative dosage, dosages of pesticide from each food source and exposure route, and the current average concentration of pesticide in the animal group biomass. Also written to this file is mass balance error for the entire food chain. This term is computed by summing the mass of pesticide taken up by all animals and subtracting losses due to decay and depuration. The value of the mass balance error indicates the relative magnitude of numerical and round off errors, and serves as an internal consistency check on the APUM module.

The second APUM output file is a time series file containing daily values of various user-specified parameters, and is formatted for use by plotting and spreadsheet software packages. This file is similar in format to the time series file produced by TFAT. Each row in the time series file contains 1) the date, 2) the Julian day, and 3) NPLTS entries of user-selected output parameters. Output parameters which may be selected include the following:

- Cumulative pesticide dosage (mg/mg)
- Concentration of pesticide in animals (mg/mg)
- Lethal dosages (mg/mg)
- Upper and lower bounds on lethal dosages (mg/mg)

Figure 7.11 shows an example APUM time series file.



```
|****************************
* MONTHLY ECOSYSTEM STATUS *
* HABITAT  1               *
*                          *
* DATE:    31 MAY., 50     *
****************************

                         ALL HYDROLOGY UNITS ARE CM OF WATER
                         SEDIMENT UNITS ARE METRIC TONNES
                         NUMBERS IN PARENTHESES ARE SOIL WATER CONTENTS

CURRENT CONDITIONS
------------------

CROP NUMBER                                1
FRACTION OF GROUND COVER              0.2990
ABOVE GROUND BIOMASS (KG/M^2)         0.3185
ROOT BIOMASS (KG/M^2)                 0.1766
ROOTING DEPTH (CM)                     25.21
LEAF AREA INDEX                        1.334
CROP YIELD (KG/M^2)                   0.2125
CANOPY HEIGHT (M)                     0.2201
INTERCEPTION POTENTIAL (CM)           0.4485E-01
DEPTH TO WHICH ET EXTRACTED(CM)        35.00


WATER FLUXES AND STORAGES FOR THIS PERIOD
-----------------------------------------


                     PREVIOUS
                     STORAGE      PRECIPITATION   EVAPORATION   THROUGHFALL   CURRENT
CANOPY                                                                        STORAGE
                     0.0000E+00   8.610           0.1733        8.437
                                                                              0.0000E+00

                     PREVIOUS
                     STORAGE      THROUGHFALL
                                                                EVAPORATION   INFILTRATION   RUNOFF     CURRENT
SURFACE PONDS        0.0000E+00   8.437                                                                 STORAGE
                                                                0.0000E+00    7.493          0.9434
                                                                                                        0.0000E+00

SOIL LAYERS          PREVIOUS              LEACHING                     LEACHING      CURRENT
HORIZON  COMPARTMENT STORAGE               INPUT       TRANSPIRATION    OUTPUT        STORAGE
-----------------------------------------------------------------------------------------------------

   1        1        0.7812   (.156)      7.493       1.187            6.329         0.7586   (.152)
   1        2        0.7541   (.151)      6.329       0.8423           5.727         0.5134   (.103)
   1        3        0.7638   (.153)      5.727       0.7156           5.248         0.5277   (.106)
   1        4        0.9259   (.185)      5.248       0.8107           4.805         0.5578   (.112)

   2        5        0.7408   (.148)      4.805       0.5833           4.360         0.6023   (.120)
   2        6        0.6273   (.125)      4.360       0.3964           3.908         0.6823   (.136)
   2        7        0.7690   (.154)      3.909       0.2783           3.576         0.8220   (.164)
   2        8        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2        9        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       10        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       11        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       12        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       13        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       14        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       15        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       16        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       17        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       18        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       19        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)
   2       20        1.000    (.200)      3.576       0.0000E+00       3.576         1.000    (.200)

SUMMARY FLUXES
--------------

TOTAL SEDIMENT ERODED FROM SURFACE   0.0000E+00
TOTAL ET FROM PROFILE                 4.815
RECHARGE BELOW ROOT ZONE              3.576
```

Figure 7.6. Example of habitat hydrologic status output.

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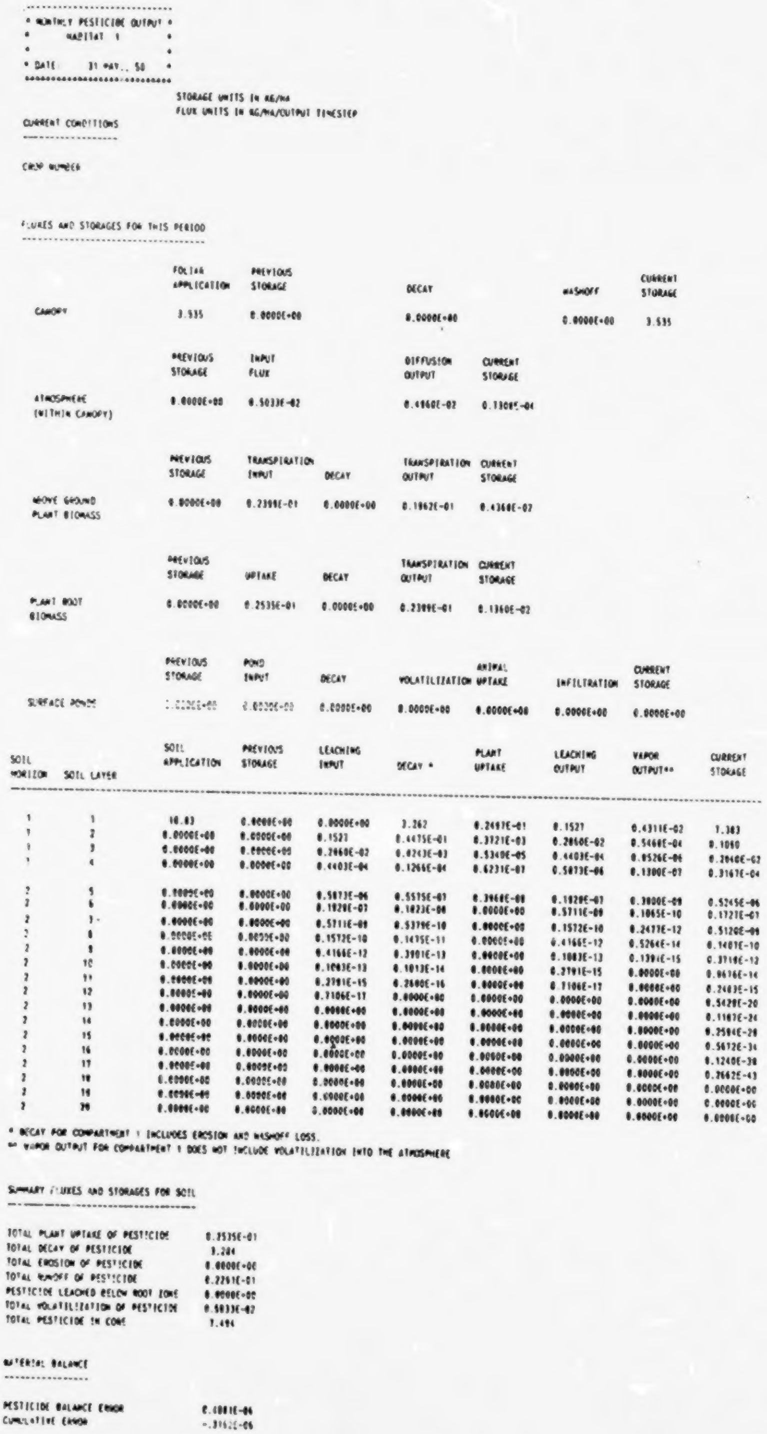
best available copy.



```
**************************
* MONTHLY PESTICIDE OUTPUT *
*       HABITAT  1         *
*                          *
* DATE:     31 MAY., 50    *
****************************
                          STORAGE UNITS IN KG/HA
                          FLUX UNITS IN KG/HA/OUTPUT TIMESTEP
CURRENT CONDITIONS
------------------

CROP NUMBER


FLUXES AND STORAGES FOR THIS PERIOD
-----------------------------------

                     FOLIAR       PREVIOUS                                              CURRENT
                     APPLICATION  STORAGE                 DECAY               WASHOFF   STORAGE

  CANOPY              3.535       0.0000E+00              0.0000E+00          0.0000E+00  3.535

                     PREVIOUS     INPUT                   DIFFUSION  CURRENT
                     STORAGE      FLUX                    OUTPUT     STORAGE

  ATMOSPHERE         0.0000E+00   0.5033E-02              0.4960E-02 0.1308E-04
  (WITHIN CANOPY)

                     PREVIOUS     TRANSPIRATION           TRANSPIRATION CURRENT
                     STORAGE      INPUT        DECAY      OUTPUT        STORAGE

  ABOVE GROUND       0.0000E+00   0.2399E-01   0.0000E+00 0.1962E-01    0.4360E-02
  PLANT BIOMASS

                     PREVIOUS                             TRANSPIRATION CURRENT
                     STORAGE      UPTAKE       DECAY      OUTPUT        STORAGE

  PLANT ROOT         0.0000E+00   0.2535E-01   0.0000E+00 0.2399E-01    0.1360E-02
  BIOMASS

                     PREVIOUS     POND                                  ANIMAL                    CURRENT
                     STORAGE      INPUT        DECAY      VOLATILIZATION UPTAKE     INFILTRATION  STORAGE

  SURFACE PONDS      0.0000E+00   0.0000E+00   0.0000E+00 0.0000E+00    0.0000E+00  0.0000E+00    0.0000E+00

SOIL                 SOIL         PREVIOUS     LEACHING                PLANT       LEACHING    VAPOR       CURRENT
HORIZON  SOIL LAYER  APPLICATION  STORAGE      INPUT       DECAY *     UPTAKE      OUTPUT      OUTPUT**    STORAGE
-------------------------------------------------------------------------------------------------------------------

   1        1         10.83       0.0000E+00   0.0000E+00   3.262      0.2497E-01  0.1527      0.4311E-02   7.383
   1        2        0.0000E+00   0.0000E+00   0.1527      0.4475E-01  0.3721E-03  0.2860E-02  0.5460E-04  0.1050
   1        3        0.0000E+00   0.0000E+00   0.2860E-02  0.8243E-03  0.5340E-05  0.4403E-04  0.8526E-06  0.2040E-02
   1        4        0.0000E+00   0.0000E+00   0.4403E-04  0.1266E-04  0.6231E-07  0.5873E-06  0.1300E-07  0.3167E-04

   2        5        0.0000E+00   0.0000E+00   0.5873E-06  0.5515E-07  0.3960E-08  0.1828E-07  0.3800E-09  0.5245E-06
   2        6        0.0000E+00   0.0000E+00   0.1828E-07  0.1823E-08  0.0000E+00  0.5711E-09  0.1065E-10  0.1727E-07
   2        7        0.0000E+00   0.0000E+00   0.5711E-09  0.5379E-10  0.0000E+00  0.1572E-10  0.2477E-12  0.5120E-09
   2        8        0.0000E+00   0.0000E+00   0.1572E-10  0.1475E-11  0.0000E+00  0.4166E-12  0.5264E-14  0.1401E-10
   2        9        0.0000E+00   0.0000E+00   0.4166E-12  0.3901E-13  0.0000E+00  0.1083E-13  0.1394E-15  0.3718E-12
   2       10        0.0000E+00   0.0000E+00   0.1083E-13  0.1013E-14  0.0000E+00  0.2791E-15  0.0000E+00  0.9636E-14
   2       11        0.0000E+00   0.0000E+00   0.2791E-15  0.2600E-16  0.0000E+00  0.7106E-17  0.0000E+00  0.2483E-15
   2       12        0.0000E+00   0.0000E+00   0.7106E-17  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.5429E-20
   2       13        0.0000E+00   0.0000E+00   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.1107E-24
   2       14        0.0000E+00   0.0000E+00   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.2594E-29
   2       15        0.0000E+00   0.0000E+00   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.5672E-34
   2       16        0.0000E+00   0.0000E+00   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.1240E-38
   2       17        0.0000E+00   0.0000E+00   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.2662E-43
   2       18        0.0000E+00   0.0000E+00   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   2       19        0.0000E+00   0.0000E+00   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   2       20        0.0000E+00   0.0000E+00   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
* DECAY FOR COMPARTMENT 1 INCLUDES EROSION AND WASHOFF LOSS.
** VAPOR OUTPUT FOR COMPARTMENT 1 DOES NOT INCLUDE VOLATILIZATION INTO THE ATMOSPHERE


SUMMARY FLUXES AND STORAGES FOR SOIL
------------------------------------

TOTAL PLANT UPTAKE OF PESTICIDE        0.2535E-01
TOTAL DECAY OF PESTICIDE                3.284
TOTAL EROSION OF PESTICIDE             0.0000E+00
TOTAL RUNOFF OF PESTICIDE              0.2261E-01
PESTICIDE LEACHED BELOW ROOT ZONE      0.0000E+00
TOTAL VOLATILIZATION OF PESTICIDE      0.5033E-02
TOTAL PESTICIDE IN CORE                 7.494


MATERIAL BALANCE
----------------

PESTICIDE BALANCE ERROR                0.4081E-06
CUMULATIVE ERROR                       -.3162E-06
```

Figure 7.7. Example of the habitat pesticide mass status output.

```
1PESTICIDE CONCENTRATION PROFILE - HABITAT  1

 DATE (DAY-MONTH-YEAR)    31 MAY., 50

 PESTICIDE CONCENTRATIONS IN PLANTS
 ---------------------------------

        CONC. IN ROOT BIOMASS (MG/MG)            0.7702E-06
        CONC. IN ABOVE GROUND BIOMASS (MG/MG)    0.1371E-05

 PESTICIDE CONCENTRATIONS IN LOCAL SOIL ORGANISMS
 ----------------------------------------------

                                                PEST. CONC.
                                                 (MG/MG)
        L. CASTANEUS 1                          0.1308E-04
        L. TERRESTRIS                           0.1591E-05

 PESTICIDE CONCENTRATIONS IN HABITAT-MOBILE ORGANISMS
 --------------------------------------------------

                                                PEST. CONC.
                                                 (MG/MG)
        T. MIGRATORIUS                          0.2138E-06


 SOIL PESTICIDE CONCENTRATIONS:
 ------------------------------

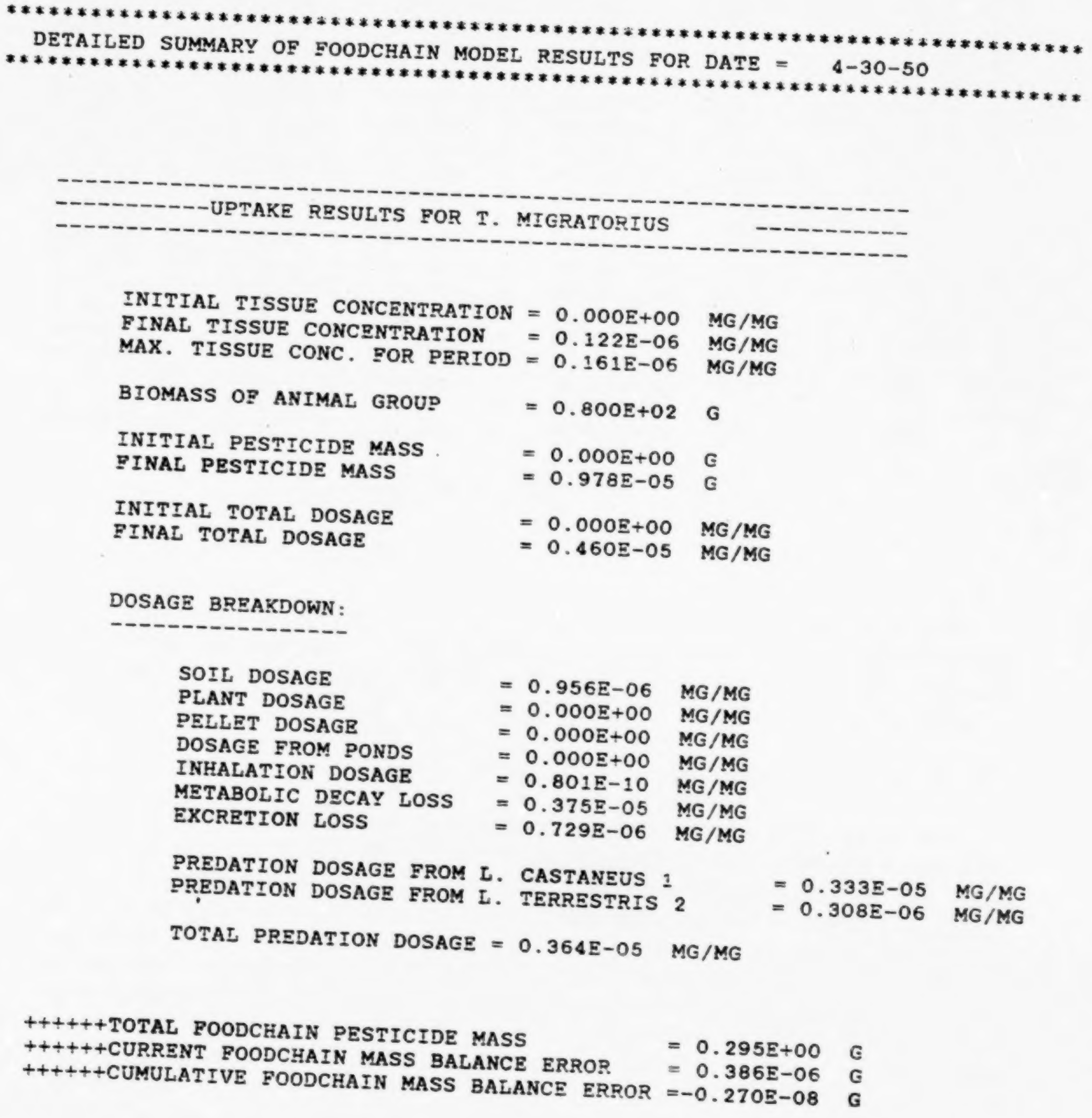
 HORIZON      COMPARTMENT        TOTAL      ADSORBED    DISSOLVED   VAPOR PHASE
                                 (MG/KG)    (MG/KG)     (MG/L)      (MG/L)
 -----------------------------------------------------------------------------

    1              1              10.18      10.15      0.3383      0.1962E-04
    1              2            0.1503     0.1500      0.4999E-02 0.2899E-06
    1              3            0.2814E-02 0.2807E-02 0.9358E-04 0.5428E-08
    1              4            0.4368E-04 0.4356E-04 0.1452E-05 0.8422E-10
    2              5            0.6768E-06 0.6715E-06 0.6715E-07 0.3895E-11
    2              6            0.2228E-07 0.2208E-07 0.2208E-08 0.1281E-12
    2              7            0.6606E-09 0.6537E-09 0.6537E-10 0.3791E-14
    2              8            0.1816E-10 0.1792E-10 0.1792E-11 0.1040E-15
    2              9            0.4798E-12 0.4737E-12 0.4737E-13 0.2748E-17
    2             10            0.1248E-13 0.1233E-13 0.1233E-14 0.7149E-19
    2             11            0.3204E-15 0.3163E-15 0.3163E-16 0.1835E-20
    2             12            0.7005E-20 0.6915E-20 0.6915E-21 0.0000E+00
    2             13            0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    2             14            0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    2             15            0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    2             16            0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    2             17            0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    2             18            0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    2             19            0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    2             20            0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
```

Figure 7.8. Example of the habitat pesticide concentration output.

```
1'TIME SERIES OUTPUT FILES'
 'HABITAT 1 ------ for DIAZINON application to peanuts, Tifton, GA          TFAT1  '
'HAB''YEAR/MO/DAY' 'JUL'    'TPST'         'TPST'          '
'---''-----------' '---'    '----'         '----'          '
   1'  1950  4  1'  91   0.00000E+00   0.00000E+00
1'TIME SERIES OUTPUT FILES'
 'HABITAT 2 ------ for DIAZINON application to peanuts, Tifton, GA          TFAT1  '
'HAB''YEAR/MO/DAY' 'JUL'    'TPST'         'TPST'          '
'---''-----------' '---'    '----'         '----'          '
   2'  1950  4  1'  91   0.00000E+00   0.00000E+00
   1'  1950  4  2'  92   0.00000E+00   0.00000E+00
   2'  1950  4  2'  92   0.00000E+00   0.00000E+00
   1'  1950  4  3'  93   0.00000E+00   0.00000E+00
   2'  1950  4  3'  93   0.00000E+00   0.00000E+00
   1'  1950  4  4'  94   0.00000E+00   0.00000E+00
   2'  1950  4  4'  94   0.00000E+00   0.00000E+00
   1'  1950  4  5'  95   0.00000E+00   0.00000E+00
   2'  1950  4  5'  95   0.00000E+00   0.00000E+00
   1'  1950  4  6'  96   0.00000E+00   0.00000E+00
   2'  1950  4  6'  96   0.00000E+00   0.00000E+00
   1'  1950  4  7'  97   0.00000E+00   0.00000E+00
   2'  1950  4  7'  97   0.00000E+00   0.00000E+00
   1'  1950  4  8'  98   0.00000E+00   0.00000E+00
   2'  1950  4  8'  98   0.00000E+00   0.00000E+00
   1'  1950  4  9'  99   0.00000E+00   0.00000E+00
   2'  1950  4  9'  99   0.00000E+00   0.00000E+00
   1'  1950  4 10' 100   0.00000E+00   0.00000E+00
   2'  1950  4 10' 100   0.00000E+00   0.00000E+00
   1'  1950  4 11' 101   0.00000E+00   0.00000E+00
   2'  1950  4 11' 101   0.00000E+00   0.00000E+00
   1'  1950  4 12' 102   0.00000E+00   0.00000E+00
   2'  1950  4 12' 102   0.00000E+00   0.00000E+00
   1'  1950  4 13' 103   0.00000E+00   0.00000E+00
   2'  1950  4 13' 103   0.00000E+00   0.00000E+00
   1'  1950  4 14' 104   0.00000E+00   0.00000E+00
   2'  1950  4 14' 104   0.00000E+00   0.00000E+00
   1'  1950  4 15' 105   0.00000E+00   0.00000E+00
   2'  1950  4 15' 105   0.00000E+00   0.00000E+00
   1'  1950  4 16' 106   0.00000E+00   0.00000E+00
   2'  1950  4 16' 106   0.00000E+00   0.00000E+00
   1'  1950  4 17' 107   0.00000E+00   0.00000E+00
   2'  1950  4 17' 107   0.00000E+00   0.00000E+00
   1'  1950  4 18' 108   0.00000E+00   0.00000E+00
   2'  1950  4 18' 108   0.00000E+00   0.00000E+00
   1'  1950  4 19' 109   0.00000E+00   0.00000E+00
   2'  1950  4 19' 109   0.00000E+00   0.00000E+00
   1'  1950  4 20' 110   0.00000E+00   0.00000E+00
   2'  1950  4 20' 110   0.00000E+00   0.00000E+00
   1'  1950  4 21' 111   0.00000E+00   0.00000E+00
   2'  1950  4 21' 111   0.00000E+00   0.00000E+00
```

Figure 7.9. Example of the habitat time series output.



```
*********************************************************************************
  DETAILED SUMMARY OF FOODCHAIN MODEL RESULTS FOR DATE =    4-30-50
*********************************************************************************


   ----------------------------------------------------------------
   -----------UPTAKE RESULTS FOR T. MIGRATORIUS      -----------
   ----------------------------------------------------------------


         INITIAL TISSUE CONCENTRATION = 0.000E+00  MG/MG
         FINAL TISSUE CONCENTRATION   = 0.122E-06  MG/MG
         MAX. TISSUE CONC. FOR PERIOD = 0.161E-06  MG/MG

         BIOMASS OF ANIMAL GROUP      = 0.800E+02  G

         INITIAL PESTICIDE MASS       = 0.000E+00  G
         FINAL PESTICIDE MASS         = 0.978E-05  G

         INITIAL TOTAL DOSAGE         = 0.000E+00  MG/MG
         FINAL TOTAL DOSAGE           = 0.460E-05  MG/MG

         DOSAGE BREAKDOWN:
         -----------------

              SOIL DOSAGE          = 0.956E-06  MG/MG
              PLANT DOSAGE         = 0.000E+00  MG/MG
              PELLET DOSAGE        = 0.000E+00  MG/MG
              DOSAGE FROM PONDS    = 0.000E+00  MG/MG
              INHALATION DOSAGE    = 0.801E-10  MG/MG
              METABOLIC DECAY LOSS = 0.375E-05  MG/MG
              EXCRETION LOSS       = 0.729E-06  MG/MG

              PREDATION DOSAGE FROM L. CASTANEUS 1       = 0.333E-05  MG/MG
              PREDATION DOSAGE FROM L. TERRESTRIS 2      = 0.308E-06  MG/MG

              TOTAL PREDATION DOSAGE = 0.364E-05  MG/MG


++++++TOTAL FOODCHAIN PESTICIDE MASS                = 0.295E+00  G
++++++CURRENT FOODCHAIN MASS BALANCE ERROR          = 0.386E-06  G
++++++CUMULATIVE FOODCHAIN MASS BALANCE ERROR =-0.270E-08  G
```

Figure 7.10 APUM dosage breakdown output file.

```
  "NEW"        "JULIAN"    "CORG "       "CORG "       "DOSE "       "LD50 "
  "DATE"         "DAY"    "L. CAST"     "T. MIGR"     "T. MIGR"     "T. MIGR"
" 4- 1-50"        91     0.000E+00     0.000E+00     0.000E+00     0.000E+00
" 4- 2-50"        92     0.000E+00     0.000E+00     0.000E+00     0.000E+00
" 4- 3-50"        93     0.000E+00     0.000E+00     0.000E+00     0.000E+00
" 4- 4-50"        94     0.000E+00     0.000E+00     0.000E+00     0.000E+00
" 4- 5-50"        95     0.000E+00     0.000E+00     0.000E+00     0.000E+00
" 4- 6-50"        96     0.000E+00     0.000E+00     0.000E+00     0.000E+00
" 4- 7-50"        97     0.327E-05     0.270E-07     0.422E-07     0.000E+00
" 4- 8-50"        98     0.967E-05     0.912E-07     0.196E-06     0.000E+00
" 4- 9-50"        99     0.112E-04     0.132E-06     0.405E-06     0.000E+00
" 4-10-50"       100     0.100E-04     0.142E-06     0.615E-06     0.000E+00
" 4-11-50"       101     0.112E-04     0.148E-06     0.827E-06     0.000E+00
" 4-12-50"       102     0.117E-04     0.155E-06     0.105E-05     0.000E+00
" 4-13-50"       103     0.119E-04     0.159E-06     0.128E-05     0.000E+00
" 4-14-50"       104     0.119E-04     0.161E-06     0.151E-05     0.000E+00
" 4-15-50"       105     0.118E-04     0.161E-06     0.174E-05     0.000E+00
" 4-16-50"       106     0.116E-04     0.160E-06     0.197E-05     0.000E+00
" 4-17-50"       107     0.978E-05     0.151E-06     0.219E-05     0.000E+00
" 4-18-50"       108     0.103E-04     0.147E-06     0.239E-05     0.000E+00
" 4-19-50"       109     0.892E-05     0.140E-06     0.259E-05     0.000E+00
" 4-20-50"       110     0.809E-05     0.131E-06     0.277E-05     0.000E+00
" 4-21-50"       111     0.907E-05     0.131E-06     0.296E-05     0.000E+00
```

Figure 7.11 APUM time series output file.

Note that during Monte Carlo simulation the APUM output files are not produced due to the potentially large amount of information that would otherwise be written out. See the Monte Carlo output description for information on Monte Carlo output.

7.6 MCARLO

The Monte Carlo module produces two output files, including a summary file and a parameter file. Note that for variables which vary in time the Monte Carlo module performs statistics on maximum moving averages of specified length. Thus, if the user specifies a 5-day averaging period the model will select the maximum 5-day average value from each Monte Carlo run for statistical calculations. The summary file contains summary statistics, correlations, and cumulative distributions for the Monte Carlo simulation. For each user-selected output variable the Monte Carlo module writes out the mean, standard deviation, skewness coefficient, minimum, and maximum over all Monte Carlo runs. Also written out is a correlation matrix containing the value of the correlation for each pair of selected output variables. Finally, the summary file contains tables and line plots of cumulative distributions for a selected subset of output variables. Figure 7.12 illustrates an example Monte Carlo summary output file.

```
      M O N T E - C A R L O   O U T P U T
      -----------------------------------
    'NOTE THAT VALUES ARE MAXIMUM N-DAY MOVING AVERAGES'
    '(I.E. MAX. AVERAGE DAILY VALUES OVER N-DAY PERIODS)'




SUMMARY STATISTICS OVER ALL MONTE-CARLO RUNS
FOR SELECTED VARIABLES:
---------------------------------------------


VARIABLE         INDEX  AVERAGING  MEAN     STANDARD   COEFF. OF   SKEW    MINIMUM    MAXIMUM
                        PER.(DAYS)          DEVIATION  VARIATION  COEFF.
---------------------------------------------------------------------------------------------
SOIL BULK DENS     1       1        1.49    0.104      0.702E-01 0.279      1.33       1.70
SOIL BULK DENS     2       1        1.54    0.802E-01 0.519E-01-0.250       1.35       1.70
BCF                2       1        5.00    0.000E+00 0.000E+00 0.000E+00  5.00       5.00
SOIL PESTICIDE     1       5        7.06    0.885E-03 0.125E-03-0.361E+04  7.06       7.06
ORG PEST CONC/     2      15   0.176E-05 0.174E-06 0.991E-01-0.906        0.134E-05 0.205E-05
ORG PEST CONC/     3       1   0.526E-06 0.130E-06 0.246      -0.279E-01 0.289E-06 0.733E-06


CORRELATION MATRIX FOR SUMMARY OUTPUT VARIABLES:
------------------------------------------------


                       SOIL    SOIL    BCF     SOIL    ORG P   ORG P

 SOIL BULK DENSITY     1.000   0.342   0.000   0.996  -0.808  -0.997

 SOIL BULK DENSITY     0.342   1.000   0.000   0.383  -0.170  -0.371

 BCF                   0.000   0.000   1.000   0.000   0.000   0.000

 SOIL PESTICIDE        0.996   0.383   0.000   1.000  -0.778  -0.999

 ORG PEST CONC/ANIM   -0.808  -0.170   0.000  -0.778   1.000   0.788

 ORG PEST CONC/ANIM   -0.997  -0.371   0.000  -0.999   0.788   1.000
```

Figure 7.12 Monte Carlo summary output file.

```
CUMULATIVE DISTRIBUTION FOR ORG PEST CONC/ANIM[3]
-----------------------------------------------------


               N                        =    20
               MEAN                     =  0.526E-06
               STANDARD DEVIATION       =  0.130E-06
               COEFFICIENT OF VARIATION =  0.246
               MINIMUM VALUE            =  0.289E-06
               MAXIMUM VALUE            =  0.733E-06
               80th PERCENTILE          =  0.654E-06
               85th PERCENTILE          =  0.657E-06
               90th PERCENTILE          =  0.713E-06
               95th PERCENTILE          =  0.724E-06
----------------------------------------------------------

  VALUE       % OF TIME EQUALLED  % OF TIME IN INTERVAL
                 OR EXCEEDED
----------------------------------------------------------

 0.289E-06       100.000
                                      10.000
 0.334E-06        90.000
                                       0.000
 0.378E-06        90.000
                                      15.000
 0.422E-06        75.000
                                       5.000
 0.467E-06        70.000
                                      10.000
 0.511E-06        60.000
                                      30.000
 0.556E-06        30.000
                                       0.000
 0.600E-06        30.000
                                       5.000
 0.645E-06        25.000
                                      10.000
 0.689E-06        15.000
                                      10.000
 0.733E-06         5.000
----------------------------------------------------------
```

Figure 7.12 Monte Carlo summary output file (continued).

```
C 100 +------+------+------+------+------+------+------+------+------+------+
U     !                                                                     **
M     !                                                                   ** !
U     !                                                          *********   !
L  80 +------+------+------+------+------+------+------+------+------+------+
A     !                                                   *******            !
T     !                                         **********                   !
I     !                                                                      !
V  60 +------+------+------+------+------+------+------+------+------+------+
E     !                                       *                              !
      !                                    ***                               !
F     !                                                                      !
R  40 +------+------+------+------+--******-----+------+------+------+------+
E     !                             *                                        !
Q     !                         ****                                         !
U     !                 ********                                             !
E  20 +------+------+------+------+------+------+------+------+------+------+
N     !              ***                                                     !
C     !     *********                                                        !
Y     !*****                                                                 !
    0 +------+------+------+------+------+------+------+------+------+------+
    0.289  0.334  0.378  0.422  0.467  0.511  0.556  0.600  0.645  0.689  0.733
                                 *  0.1E-05

                                ORG PEST CONC/ANIM[3]
```

Figure 7.12 Monte Carlo summary output file (concluded).

The second Monte Carlo output file contains the values of variables for each Monte Carlo run. The user selects which variables are to be written to this file in column format. The data in this file can be used to plot cumulative distributions and to examine the combinations of input variables which produce various model results. An example of this file is shown in Figure 7.13.

```
          "MODEL PARAMETERS FOR EACH MONTE-CARLO RUN:"

          "NOTE THAT VALUES ARE MAXIMUM N-DAY MOVING AVERAGES"
          "(I.E. MAX. AVERAGE DAILY VALUES OVER N-DAY PERIODS)"


"RUN NO"   "SOIL BULK DEN"   "SOIL BULK DEN"    "ORG PEST CONC"
                  1                 2                  3
"------"   "-------------"   "-------------"    "-------------"
     1         1.520             1.538            0.4751E-06
     2         1.466             1.567            0.5406E-06
     3         1.328             1.505            0.7335E-06
     4         1.382             1.550            0.6569E-06
     5         1.347             1.534            0.7133E-06
     6         1.657             1.575            0.3244E-06
     7         1.484             1.551            0.5196E-06
     8         1.539             1.544            0.4531E-06
     9         1.517             1.696            0.4842E-06
    10         1.459             1.663            0.5485E-06
    11         1.461             1.665            0.5448E-06
    12         1.419             1.460            0.6126E-06
    13         1.584             1.516            0.3995E-06
    14         1.461             1.464            0.5474E-06
    15         1.334             1.348            0.7245E-06
    16         1.381             1.461            0.6538E-06
    17         1.486             1.577            0.5232E-06
    18         1.695             1.503            0.2891E-06
    19         1.602             1.609            0.3822E-06
    20         1.584             1.565            0.3991E-06
```

Figure 7.13 Monte Carlo parameters output file.

SECTION 8

EXAMPLE APPLICATION

This section gives the results of a comprehensive example application so that the user can benchmark simulations on his machine. It makes use of all of the (deterministic) TEEAM modules and performs a multiple habitat simulation. It does not, however, utilize the model's Monte Carlo simulation capabilities. The problem is realistic in its assessment of physical, chemical, and biological parameters. Some license has been taken with some aspects of the system in order to gain comprehensiveness. For instance, aerial application of the chemical in the region simulated may not be a normal agricultural practice. Obviously, the avian in the simulation would eat food items in addition to the earthworms, as suggested by the input sequence.

The input files for this simulation are provided on the set of discs containing the code and are not shown in this section.

8.1 GENERAL PROBLEM SETTING

The simulation involves the estimation of exposure of diazinon to passerine birds (American Robin) in a hypothetical peanut field near Tifton, GA. Meteorological data for Tifton, GA are used. The field is square, 8 ha in size, half of which is aerially sprayed with diazinon at a rate of 1 gal acre^{-1}.

8.2 FSCBG AND GRDDEF INPUTS

Two aerial applications are simulated, one occurring on May 5 and one on May 25. The aircraft is assumed to be a Schweitzer Ag Cat. As mentioned above, the application rate is 1 gal acre^{-1}. Wind is assumed to be out of the west (270°) for both spray events. Other meteorological inputs are in the echoed output, shown later in this section.

The aircraft is assumed to make seven passes in a north-south direction on the western half of the 8 ha field (Habitat 1). Therefore, the other half of the field (Habitat 2) receives only drift from the spraying of the western half. Foliar deposition is computed using the exponential model (FILTRA = 2.5 m^2 kg^{-1}) and canopy penetration is modeled using the attenuation coefficient approach (BETA = 0.15 cm^{-1}). No evaporation or decay of the sprayed product is assumed to occur during the application event.

8.3 TFAT INPUTS

Most of the TFAT inputs are taken directly from the guidance provided in Section 6. Two habitats are simulated, as described above, each having an area of 4 ha. The soil of each is assumed to be a Tifton sandy loam with a saturated hydraulic conductivity of 4.4 cm hr^{-1}. This soil is in hydrologic soil group 'B' according to Carsel et al. (1984). The top 100 cm of the soil are simulated and the soil is assumed to have two horizons. These horizons vary in their thickness, bulk density, and pesticide degradation and adsorption properties. Water holding properties of each horizon are the same. The degradation rate in the top horizon was estimated using values found in the literature for this compound. The value for the lower soil was taken as the low end of the range given in Section 6.4.1.3.

The peanut crop is planted on April 1. It is assumed to have an interception potential of 0.15 cm and a maximum rooting depth of 60 cm.

8.4 PLTGRN AND PLTRNS INPUTS

Inputs for the peanut plant growth model were taken directly from the guidance in Williams et al. (1987) as provided in this document. The UPTKF and RW factors (plant uptake factor in TFAT and reflection coefficient in PLTRNS) were assumed to be equal and in the absence of more appropriate information, to have a value of unity.

The degradation rate in the plant was unknown and, therefore, assumed to be zero. The KP for the chemical in the plant was calculated using a KOW of 1050, which yields a nearly equivalent KOC (Chiou's method, see Section 6.4.1.3) and an organic carbon content for the plant of 30%.

8.5 APUM INPUTS

For the animal exposure module, Habitat 1 is assumed to have two species of earthworms (L. Castaneaus), a small, shallow borrowing lumbricid, and L. Terrestris, which is larger and burrows more deeply. The movement transition matrices reflect this behavior. Both species were assumed to be present in Habitat 1, while only L. Castaneaus was assumed to be present in Habitat 2. Biomasses were estimated using the guidance in Section 6. Pesticide metabolic degradation rates in the lower animals were taken to be the same as that for the upper soil. Lethal dosages for earthworms were taken to be on the order of 10 μg/individual as reported by Lee (1985). Thirty percent of the diet of the robin was assumed to be made up of contaminated earthworms, 10% from each species in each habitat. Clearance rates for the robin were assumed to be equivalent to those for dieldrin in thrushes calculated from the data of Jeffries and Davis (1968). This latter assumption was made due to the lack of specific information on clearance rates for diazinon in thrushes. One would expect the diazinon clearance rate to be somewhat higher given its slightly lower K_{ow} (1050 for diazinon versus 4900 for dieldrin) in the same species. However, the rates reported by Jeffries and Davis (1968) already seem high in comparison to rates for other, similar compounds in avians (see Table 6-42).

8.6 TEEAM SIMULATION RESULTS

Results of the example problem simulation are shown in the output listing which follows (Figure 8.1). Due to the stochastic method which is used to simulate animal movement, the concentrations in lower animals and simulated dosage to the birds may be slightly different in the user's simulation than the results shown in Figure 8.1. All other results should be exact with the exceptions produced by roundoff errors on different machines.

```
****************************************************************************
 DETAILED SUMMARY OF FOODCHAIN MODEL RESULTS FOR DATE =   5-31-50
****************************************************************************



 ------------------------------------------------------------
 -----------UPTAKE RESULTS FOR L. CASTANEUS 1      -----------
 ------------------------------------------------------------


     INITIAL TISSUE CONCENTRATION = 0.000E+00  MG/MG
     FINAL TISSUE CONCENTRATION   = 0.134E-04  MG/MG
     MAX. TISSUE CONC. FOR PERIOD = 0.159E-04  MG/MG

     BIOMASS OF ANIMAL GROUP      = 0.480E+06  G

     INITIAL PESTICIDE MASS       = 0.000E+00  G
     FINAL PESTICIDE MASS         = 0.646E+01  G

     INITIAL TOTAL DOSAGE         = 0.000E+00  MG/MG
     FINAL TOTAL DOSAGE           = 0.165E-03  MG/MG

     + + + + LD-50 HAS BEEN EXCEEDED


     DOSAGE BREAKDOWN:
     -----------------

         SOIL DOSAGE            = 0.165E-03  MG/MG
         PLANT DOSAGE           = 0.000E+00  MG/MG
         PELLET DOSAGE          = 0.000E+00  MG/MG
         DOSAGE FROM PONDS      = 0.000E+00  MG/MG
         INHALATION DOSAGE      = 0.000E+00  MG/MG
         METABOLIC DECAY LOSS   = 0.152E-03  MG/MG
         EXCRETION LOSS         = 0.000E+00  MG/MG

         PREDATION DOSAGE FROM L. TERRESTRIS        = 0.000E+00  MG/MG
         PREDATION DOSAGE FROM L. CASTANEUS 2       = 0.000E+00  MG/MG
         PREDATION DOSAGE FROM T. MIGRATORIUS       = 0.000E+00  MG/MG

         TOTAL PREDATION DOSAGE = 0.000E+00  MG/MG
```

Figure 8.1. TEEAM output for the example application

```
------------------------------------------------------------
-----------UPTAKE RESULTS FOR L. TERRESTRIS       -----------
------------------------------------------------------------


     INITIAL TISSUE CONCENTRATION = 0.000E+00  MG/MG
     FINAL TISSUE CONCENTRATION   = 0.169E-05  MG/MG
     MAX. TISSUE CONC. FOR PERIOD = 0.169E-05  MG/MG

     BIOMASS OF ANIMAL GROUP      = 0.480E+06  G

     INITIAL PESTICIDE MASS       = 0.000E+00  G
     FINAL PESTICIDE MASS         = 0.810E+00  G

     INITIAL TOTAL DOSAGE         = 0.000E+00  MG/MG
     FINAL TOTAL DOSAGE           = 0.213E-05  MG/MG

     + + + + LD-10 HAS BEEN EXCEEDED


     DOSAGE BREAKDOWN:
     -----------------

          SOIL DOSAGE            = 0.213E-05  MG/MG
          PLANT DOSAGE           = 0.000E+00  MG/MG
          PELLET DOSAGE          = 0.000E+00  MG/MG
          DOSAGE FROM PONDS      = 0.000E+00  MG/MG
          INHALATION DOSAGE      = 0.000E+00  MG/MG
          METABOLIC DECAY LOSS   = 0.436E-06  MG/MG
          EXCRETION LOSS         = 0.000E+00  MG/MG

          PREDATION DOSAGE FROM L. CASTANEUS 1        = 0.000E+00  MG/MG
          PREDATION DOSAGE FROM L. CASTANEUS 2        = 0.000E+00  MG/MG
          PREDATION DOSAGE FROM T. MIGRATORIUS        = 0.000E+00  MG/MG

          TOTAL PREDATION DOSAGE = 0.000E+00  MG/MG
```

Figure 8.1. TEEAM output for the example application (continued).

```
-------------------------------------------------------------
----------UPTAKE RESULTS FOR L. CASTANEUS 2       -----------
-------------------------------------------------------------


    INITIAL TISSUE CONCENTRATION = 0.000E+00  MG/MG
    FINAL TISSUE CONCENTRATION   = 0.433E-05  MG/MG
    MAX. TISSUE CONC. FOR PERIOD = 0.433E-05  MG/MG

    BIOMASS OF ANIMAL GROUP      = 0.480E+06  G

    INITIAL PESTICIDE MASS       = 0.000E+00  G
    FINAL PESTICIDE MASS         = 0.208E+01  G

    INITIAL TOTAL DOSAGE         = 0.000E+00  MG/MG
    FINAL TOTAL DOSAGE           = 0.415E-04  MG/MG

    + + + + LD-50 HAS BEEN EXCEEDED


    DOSAGE BREAKDOWN:
    ----------------


        SOIL DOSAGE            = 0.415E-04  MG/MG
        PLANT DOSAGE           = 0.000E+00  MG/MG
        PELLET DOSAGE          = 0.000E+00  MG/MG
        DOSAGE FROM PONDS      = 0.000E+00  MG/MG
        INHALATION DOSAGE      = 0.000E+00  MG/MG
        METABOLIC DECAY LOSS   = 0.371E-04  MG/MG
        EXCRETION LOSS         = 0.000E+00  MG/MG

        PREDATION DOSAGE FROM L. CASTANEUS 1       = 0.000E+00  MG/MG
        PREDATION DOSAGE FROM L. TERRESTRIS        = 0.000E+00  MG/MG
        PREDATION DOSAGE FROM T. MIGRATORIUS       = 0.000E+00  MG/MG

        TOTAL PREDATION DOSAGE = 0.000E+00  MG/MG
```

Figure 8.1. TEEAM output for the example application (continued).

```
-------------------------------------------------------------
-----------UPTAKE RESULTS FOR T. MIGRATORIUS       -----------
-------------------------------------------------------------


    INITIAL TISSUE CONCENTRATION = 0.000E+00  MG/MG
    FINAL TISSUE CONCENTRATION   = 0.238E-06  MG/MG
    MAX. TISSUE CONC. FOR PERIOD = 0.248E-06  MG/MG

    BIOMASS OF ANIMAL GROUP      = 0.536E+04  G

    INITIAL PESTICIDE MASS       = 0.000E+00  G
    FINAL PESTICIDE MASS         = 0.128E-02  G

    INITIAL TOTAL DOSAGE         = 0.000E+00  MG/MG
    FINAL TOTAL DOSAGE           = 0.648E-05  MG/MG


    DOSAGE BREAKDOWN:
    -----------------

        SOIL DOSAGE            = 0.977E-06  MG/MG
        PLANT DOSAGE           = 0.000E+00  MG/MG
        PELLET DOSAGE          = 0.000E+00  MG/MG
        DOSAGE FROM PONDS      = 0.000E+00  MG/MG
        INHALATION DOSAGE      = 0.302E-05  MG/MG
        METABOLIC DECAY LOSS   = 0.575E-05  MG/MG
        EXCRETION LOSS         = 0.496E-06  MG/MG

        PREDATION DOSAGE FROM L. CASTANEUS 1       = 0.221E-05  MG/MG
        PREDATION DOSAGE FROM L. TERRESTRIS        = 0.185E-05  MG/MG
        PREDATION DOSAGE FROM L. CASTANEUS 2       = 0.836E-07  MG/MG

        TOTAL PREDATION DOSAGE = 0.248E-05  MG/MG


++++++TOTAL FOODCHAIN PESTICIDE MASS          = 0.935E+01  G
++++++CURRENT FOODCHAIN MASS BALANCE ERROR    = 0.128E-04  G
++++++CUMULATIVE FOODCHAIN MASS BALANCE ERROR = 0.333E-05  G
```

Figure 8.1. TEEAM output for the example application (concluded).

SECTION 9

MODEL ARCHITECTURE

The development of a framework for the model, both in an architectural and an implementational sense, is an important consideration. The utility of a piece of software can be judged by its ease of application in the opinion of the user and its appropriateness in solving the problem at hand. This framework has been conceived with both of these factors in mind.

The proposed spatial and temporal basis for the model is designed to meet the resolution required by a management-level or regulatory application. The architecture of the model hopefully balances the capability to apply computational modules in various combinations (to achieve optimal flexibility in simulating generalized ecosystems) with simplicity at the user interfaces (inputs and outputs). The design is modular so that computational modules may be added or exchanged following initial development with relative ease.

The model is designed for use on an IBM PC compatible running MS DOS. A significant feature in this regard is the size of the code. To be compatible with the 640K byte working memory limitations of most machines of this type, the code makes use of code overlays. The code also uses scratch files (as opposed to working memory) to save information to "restart" habitats when making multiple habitat simulations and to initialize Monte Carlo runs.

This section is organized in the following way. Section 9.1 discusses code architecture, including operation sequences and module content. Section 9.2 describes intermodule communication and Section 9.3, coding conventions. Section 9.4 discusses the use of files to store and transfer information critical to model operation.

9.1 CODE ARCHITECTURE

The TEEAM code consists of over 150 subroutines organized into 11 modules. Of the 11 modules, 5 perform computations; the others initialize data, perform I/O functions or provide generalized services to other parts of the code. The modules are (in alphabetical order):

APUM - Computes Pesticide Exposure to Terrestrial Animals

FSCBG - Performs Pesticide Spray Application Deposition Calculations

INPREA - Performs Program Input Functions

INITEM - Initializes Program Variables

MCARLO - Executes Monte Carlo Simulations

PLTGRN - Performs Plant Growth Computations

PLTRNS - Performs Plant Uptake and Translocation Calculations

SPECIO - Performs Specialized Output Functions

TEEAMAIN - Main Program Which Controls Input and Program Execution

UTIL - Contains Program Utility Subroutine

Table 9-1 lists each module and lists and describes the function of each subroutine it contains. Due to its length, this table appears at the end of this section. The modules are directed by an execution supervision (EXESUP). EXESUP in turn receives its instructions from BATENT, the batch input processor and ultimately from TEEAM, the main program.

A flow diagram of the TEEAM main program is given in Figure 9.1 The purpose of the main program is to determine, by reading the run file, the various options selected. TEEAM version 1.1 can currently only operate in the batch mode through the subroutine BATENT. The main program passes control to BATENT for reading data and thence to the execution supervisor. The structure of BATENT is depicted in Figure 9.2

The execution supervisor (EXESUP) is the main controlling code for TEEAM. This subroutine plus those depicted in Figures 9.1 and 9.2 comprise the module TEEAMAIN. The structure of EXESUP is depicted in Figure 9.3.

Within EXESUP there are four major loops:

- Monte Carlo
- Year
- Day
- Habitat

Within the habitat loop TFAT, PLTGRN and PLTRNS are called each day. FSCBG and GRDDEP are called from within the day loop if a spray application is indicated. APUM is also called outside the compartment loop. This is because the concentrations in the various media (soil, plants, air, etc.) need to be known for all habitats before the animal exposures can be calculated. The daily loop runs inside a year loop if the simulation extends over several years. Currently, long-term simulations are not recommended because of the inability of the code to handle seasonal aspects of animal behavior. Finally, the entire deterministic model is situated

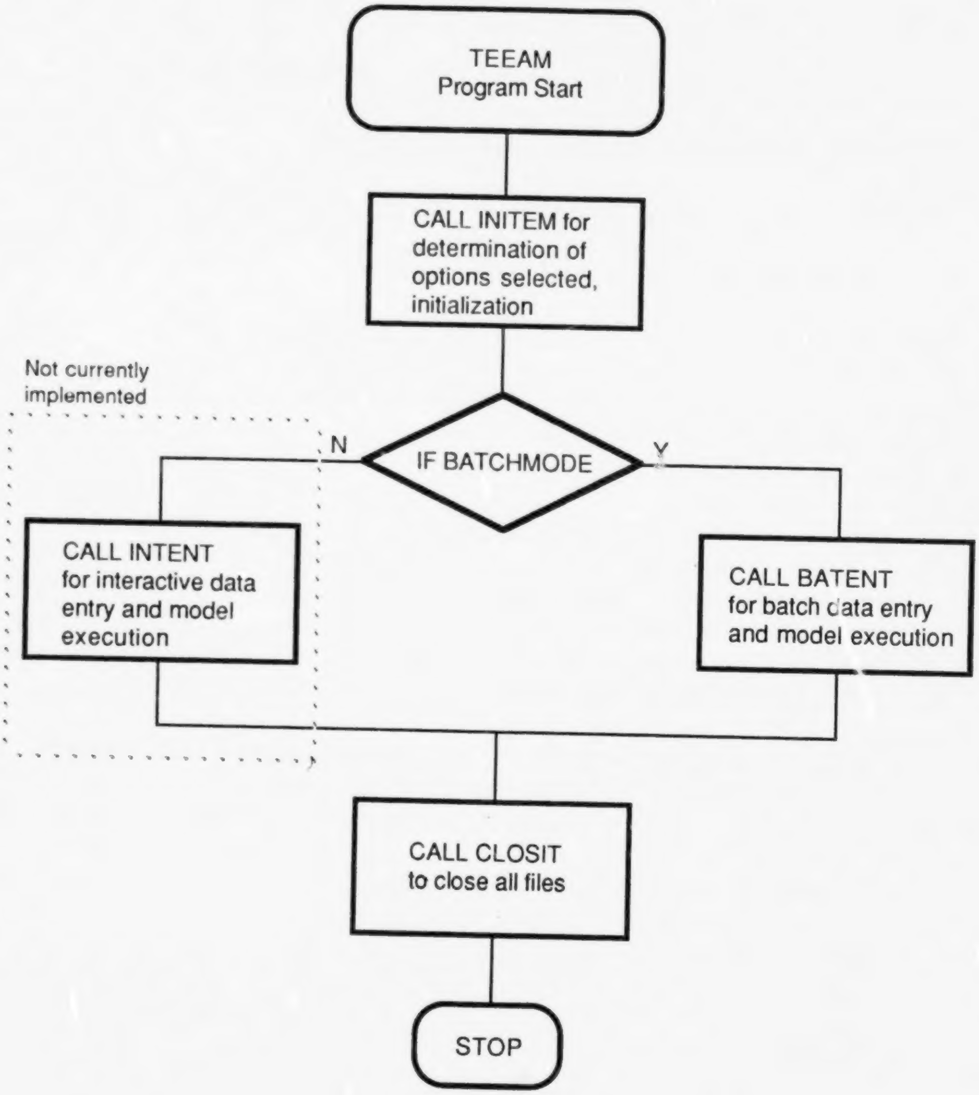

TEEAM Program Start
CALL INITEM for determination of options selected, initialization
Not currently implemented
N
IF BATCHMODE
Y
CALL INTENT for interactive data entry and model execution
CALL BATENT for batch data entry and model execution
CALL CLOSIT to close all files
STOP

Figure 9.1. TEEAM main program structure.

inside the Monte Carlo loop. Inside the Monte Carlo loop, random number generators produce probabilistic realizations of input parameter sets. In this mode, the deterministic model is run a number of times, and frequency distributions of various model outputs can be generated.

Figure 9.4 shows a schematic representation of the operation sequence shown in Figures 9.1 through 9.3, including the names of the subroutines actually called within that sequence.

The text that follows describes the structure of computational modules and includes documentation for the subroutines within each module. Modules that perform only reading, initialization, output, and general utility functions are not covered.

9.1.1 Pesticide Application/Deposition

The models for describing the application and subsequent transport and deposition of pesticides are incorporated into the FSCBG and GRDDEP modules. The pesticide spraying model is a modified version of FSCBG. The

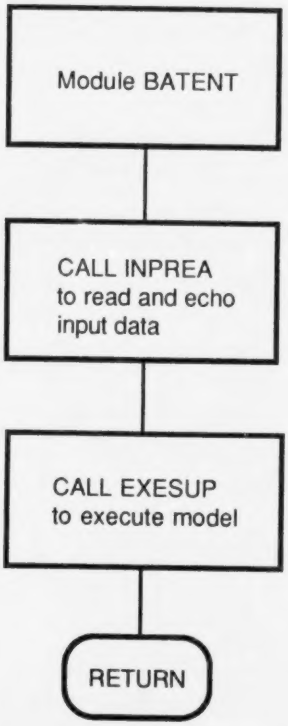


Figure 9.2. Batch input module (BATENT) structure.

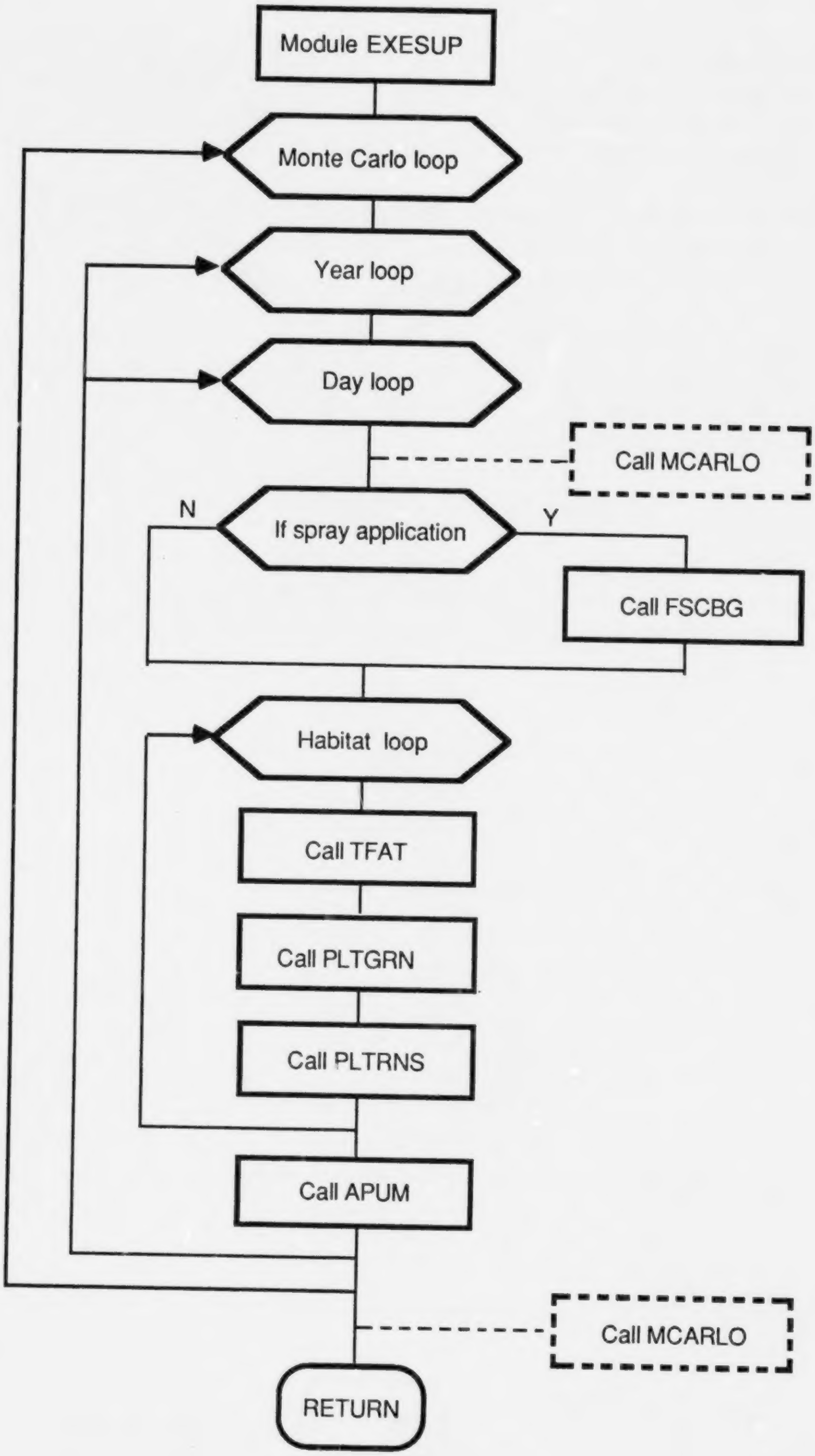

Module EXESUP
Monte Carlo loop
Year loop
Day loop
Call MCARLO
N
If spray application
Y
Call FSCBG
Habitat loop
Call TFAT
Call PLTGRN
Call PLTRNS
Call APUM
Call MCARLO
RETURN

Figure 9.3. Execution supervisor (EXESUP) structure.

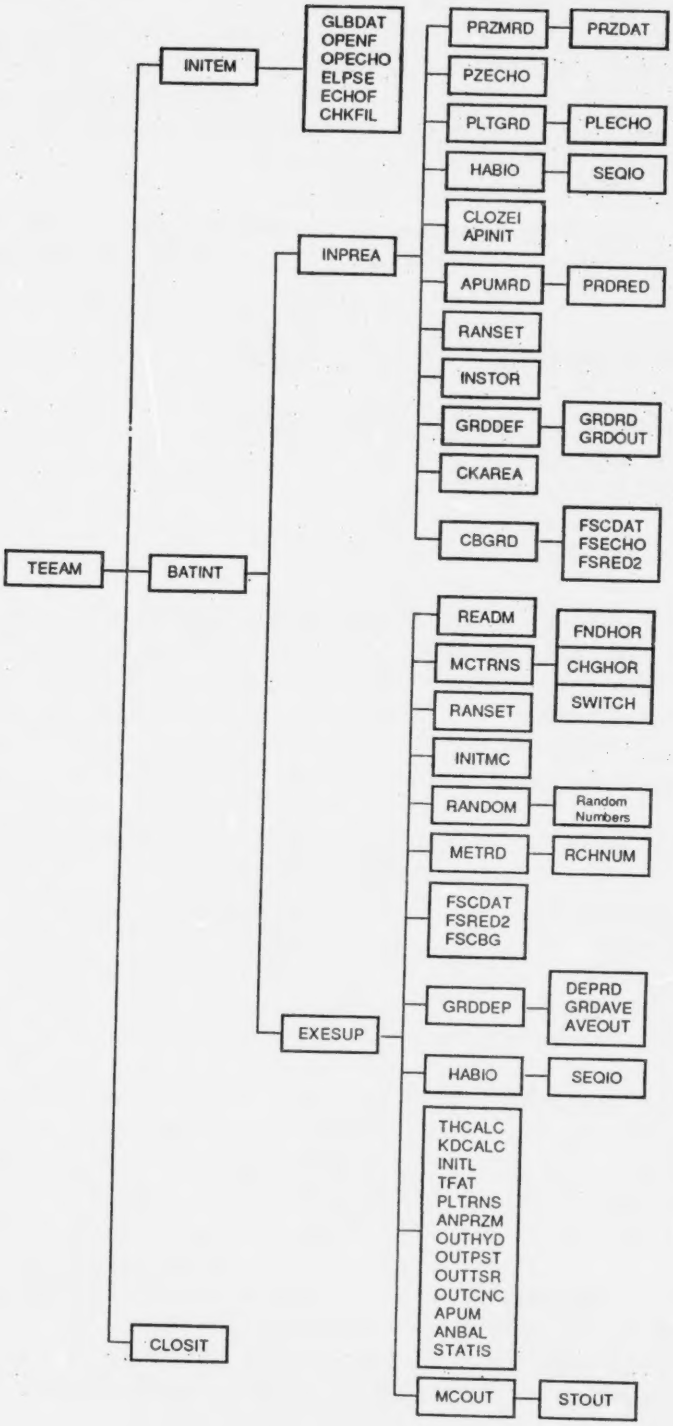

TEEAM
INITEM
GLBDAT
OPENF
OPECHO
ELPSE
ECHOF
CHKFIL
BATINT
INPREA
PRZMRD
PRZDAT
PZECHO
PLTGRD
PLECHO
HABIO
SEQIO
CLOZEI
APINIT
APUMRD
PRDRED
RANSET
INSTOR
GRDDEF
GRDRD
GRDOUT
CKAREA
CBGRD
FSCDAT
FSECHO
FSRED2
EXESUP
READM
MCTRNS
FNDHOR
CHGHOR
SWITCH
RANSET
INITMC
RANDOM
Random Numbers
METRD
RCHNUM
FSCDAT
FSRED2
FSCBG
GRDDEP
DEPRD
GRDAVE
AVEOUT
HABIO
SEQIO
THCALC
KDCALC
INITL
TFAT
PLTRNS
ANPRZM
OUTHYD
OUTPST
OUTTSR
OUTCNC
APUM
ANBAL
STATIS
MCOUT
STOUT
CLOSIT

Figure 9.4 TEEAMAIN program structure.

GRDDEP module is comprised of subroutines which link the FSCBG outputs to TEEAM. These modules are called whenever a pesticide spray event is simulated. The user should be aware that pesticide can be applied directly into habitats at specified rates in the TFAT input sequence. FSCBG/GRDDEP would be used primarily if the user is interested in quantifying drift of the spray to nontarget habitats.

9.1.1.1 FSCBG. The FSCBG program, as implemented for use with the TEEAM model, consists of three functional components (each implemented as one or more subroutines):

- Wake-Settling Velocity Model (CBGS3)
- Spray Dispersion Model (CBGS6, CBGS7)
  - dosage submodel
  - deposition submodel
- Evaporation Model (CBGS4)

The model is called from EXESUP and is supplemented by several input/output routines. The model allows for the simulation of transport of sprayed material above a vegetative canopy from multiple spray lines or swaths and can be selected for use as modeling needs and data accessibility merit. Model components are briefly described below. Figure 9.5 shows the structure of the FSCBG model as implemented in TEEAM.

The Wake-Settling Velocity submodel permits the user either to input the aircraft wake-settling velocity directly or to input the aircraft weight, wing span, and ground speed which the program uses to calculate the aircraft wake-settling velocity. This subroutine models the growth and position of the pesticide cloud, during the short period immediately after release when its shape is primarily controlled by the aircraft vortices. For ground spraying applications, this component is not used.

There are two submodels within the spray dispersion model. The user has the option of utilizing the dosage and/or deposition submodels. The submodels can be used to calculate dosage and deposition from a nearly instantaneous elevated line source oriented at an arbitrary angle with respect to the mean wind direction. These submodels will, if selected by the user, calculate the dosage and/or deposition at specified heights for locations within a rectangular grid. Calculations by the submodels are restricted to below the height of elevated inversions. In its present configuration, the FSCBG computer program can calculate the dosage, and deposition at a maximum of 737 receptor nodes downwind from a maximum of 100 line sources.

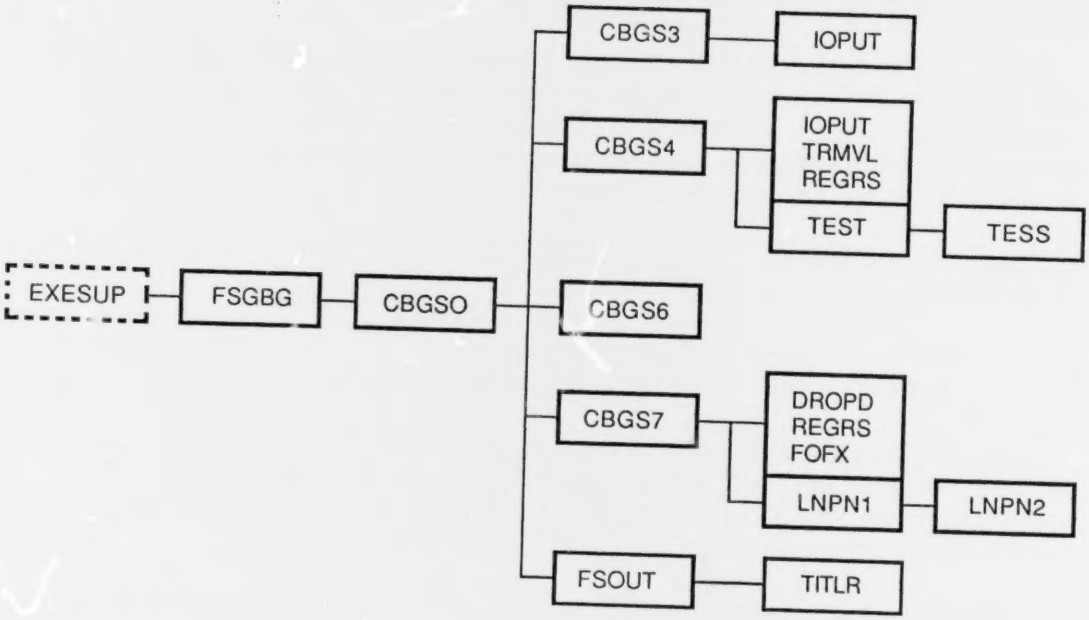

CBGS3
IOPUT
CBGS4
IOPUT
TRMVL
REGRS
TEST
TESS
EXESUP
FSGBG
CBGSO
CBGS6
CBGS7
DROPD
REGRS
FOFX
LNPN1
LNPN2
FSOUT
TITLR

Figure 9.5 Module FSCBG structure.

Evaporation is a significant mechanism by which drop-size distribution changes in time. The evaporation model allows the user to specify whether or not drop evaporation is to be included in a calculation of dosage or deposition. If the user selects a drop evaporation option, the program automatically calculates the change in drop diameter with time, using a polynomial expression fitted either to empirical data or theoretical calculations.

The canopy penetration model available in FSCBG is not used for this version of the TEEAM model. In its place a simplified canopy penetration model is used.

9.1.1.2 GRDDEP. GRDDEP consists of three subroutines which are called from EXESUP if a spray event has occurred on a given simulation day. Subroutine GRDRD is called to read the FSCBG output file which contains the deposition values at each receptor grid point. Subroutine GRDAVE then averages the deposition values within each habitat and subroutine AVEOUT writes the GRDAVE output.

9.1.2 Terrestrial Fate and Transport

The TFAT module performs terrestrial fate and transport computations. TFAT has been designed as a modular subprogram such that each important computational step is contained in a separate subroutine. Central to the module is a main subroutine or driver program (subroutine TFAT). This program calls all computational subroutines.

Subroutines are grouped into two major categories by function. These functions can be generalized into those that:

- Simulate hydrologic processes
- Simulate pesticide fate and transport processes

The subroutines which work together to perform each of these functions are described briefly below. Figure 9.6 depicts the system level organization of these subroutines. The subroutines are ordered logically (as the main program would call them) within these sections.

One-dimensional soil and surface water hydraulics are modeled by a series of functional subroutines including: PLGROW, HYDROL, POND, INFIL, EVPOTR, HYDR1 or HYDR2, and EROSN. These subroutines function as a group and describe the behavior of water in the system, without regard to toxicant chemistry. Inherent in this functional demarcation is the assumption that the chemical concentrations are low enough that any effect on the physical properties of the solution are negligible.

PLGROW is called first to simulate plant growth status and calculate parameters which affect the hydrologic simulations (i.e., canopy interception). HYDROL then calculates surface hydrologic factors such as runoff, plant interception, and snowmelt. Subroutine EROSN computes the soil loss from the habitat. Potential and actual evaporation and transpiration from the plant canopy, surface ponds, and the root zone are computed in EVPOTR. A precipitation event triggers the use of subroutines INFIL and POND to simulate pond water hydraulics and infiltration on a finer-than-daily time step. INFIL estimates the infiltration capacity of the soil through time allowing POND to simulate the evolution of ephemeral surface ponds and the soil moisture profile and soil water velocity. HYDR1 or HYDR2 calculate subsurface hydrologic factors such as pore velocities and soil moisture content in each soil compartment in the absence of a precipitation event or ponded surface water.

The pesticide fate and transport subroutines activated by the application of pesticide by the toxicant application/deposition model include DEPMOD, PESTAP, GRANUL, VOLMT, CANOPY, CNCONC, PLPEST, PCHEM, SLPEST, TRDIAG, and MASBAL. Subroutine DEPMOD is called if a spray application event occurs on a given simulation day. It rearranges the pesticide application information within the habitat, inserts the information for the spray event, and then readjusts the pesticide habitat information for the habitat. If a non-spray application of chemical occurs, subroutine PESTAP is called instead. PESTAP handles direct applications of chemical to single habitats only, including soil surface, soil incorporation, and granular applications. Subroutine GRANUL then determines the chemical release rate from granules and quantity of pesticide remaining in granules. Subroutine VOLMT sets up terms for simulation of vapor phase movement and volatilization of the pesticides from the soil in the absence of surface ponding. Subroutine CANOPY computes the canopy resistance to vapor transfer out of the habitat by upwards diffusion. PCHEM simulates fate of chemical in ephemeral surface ponds and pesticide concentration in

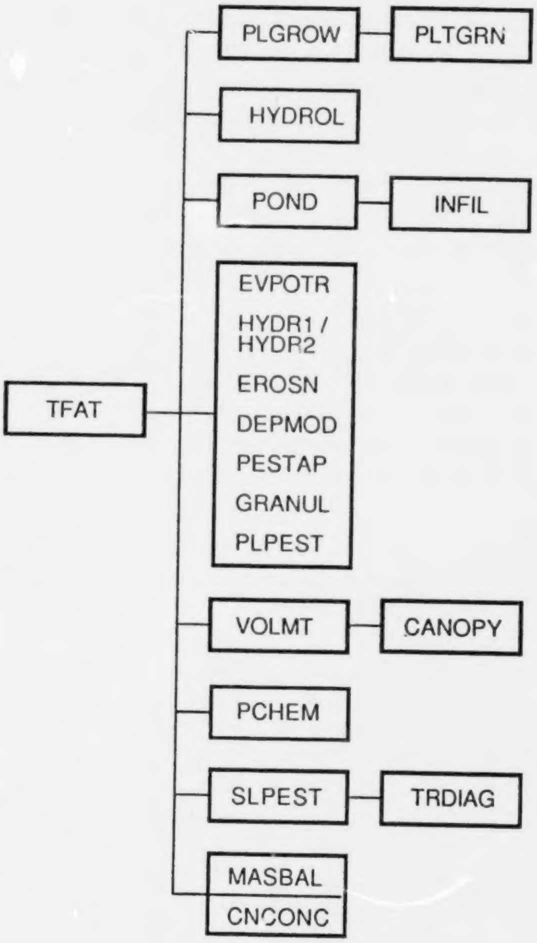

PLGROW
PLTGRN
HYDROL
POND
INFIL
EVPOTR
HYDR1 / HYDR2
EROSN
DEPMOD
PESTAP
GRANUL
PLPEST
TFAT
VOLMT
CANOPY
PCHEM
SLPEST
TRDIAG
MASBAL
CNCONC

Figure 9.6 Module TFAT structure.

the ponded water. PLPEST simulates the degradation and washoff of chemical on plant foliage. Pesticide transport through advection and dispersion, as well as the various sources and sink terms are calculated in subroutine SLPEST which predicts pesticide concentration in soil for the time step and pesticide fluxes from the soil. TRDIAG performs the Thomas algorithm to solve the tridiagonal matrix set up by SLPEST and SLTEMP. MASBAL concludes the module time step by calculating the mass balance error for water and pesticide in the system. Finally, CNCONC determines the average concentration of chemical in the atmosphere within the plant canopy.

9.1.3 Plant Growth

The alternate plant growth formulation, PLTGRN, is called as an option from the TFAT code. The structure, the linkage of the subroutines, within this module is presented in Figure 9.7. The first routine called within PLTGRN is PLTDEF, which sets up the plant growth parameters for the current plant type being simulated (the parameters for all plants in all compartments are read into arrays before EXESUP begins the simulation). The next routine, PLTDAY, computes intermediate data which are computed once each day (e.g., accumulated heat units and photosynthyetically active radiation). PLTDAY calls the routine DAYLIT to interpolate the hours of daylight for the current day. This daily datum is interpolated from the TFAT monthly daylight hour data stored in the TFAT variable DT. The actual plant growth for the day is calculated by RK4GRO. Subroutine DXGRO sets up the system of differential equations. The last routine called by PLTGRN, SAVLT, saves the results of this plant simulation into storage arrays for use when this plant is to be simulated again. Before returning control to TFAT, PLTGRN computes the value for canopy cover by using the complementary error function ERFC located in the UTIL module. At the end of PLTGRN execution, the plant growth values required by TFAT and the other modules are passed back to the TFAT subroutine, PLGROW.

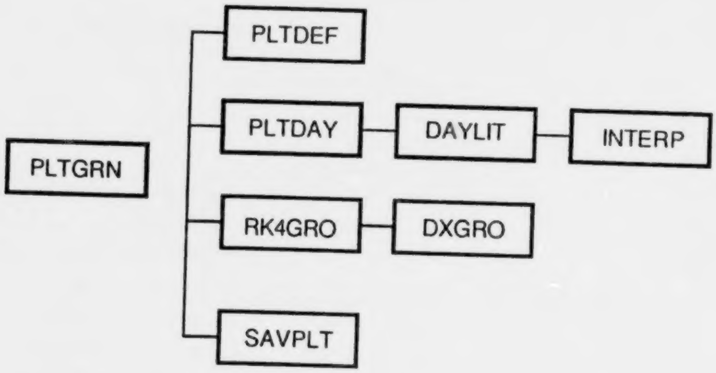


Figure 9.7 Module PLTGRN structure.

9.1.4 Plant Contaminant Transport

The structure of the plant contaminant transport module, PLTRNS (Figure 9.8), is similar to the structure of PLTGRN. The first routine called, DEFTRN, sets up the plant translocation parameters for the current plant type being simulated. The next routine called, TRNDAY, determines the daily constant data (e.g., daily transpiration rate). The daily contaminant transport within the plant is calculated by TRNDIF using a fully implicit scheme. The last routine called by PLTRNS, SAVTRN, saves the results of this plant's simulation into storage arrays for use when this plant is to be simulated again. At the end of PLTRNS execution, the plant translocation values required by the other process modules within TEEAM are stored in the appropriate common arrays.

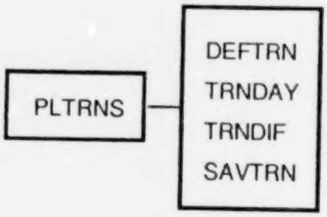


Figure 9.8 Module PLTRNS structure.

9.1.5 Terrestrial Animal Exposure

Figure 9.9 illustrates the structure of the Animal Exposure submodel. The submodel consists of three primary components:

- animal movement
- intake rate regulation
- animal feeding and toxicant assimilation

Subroutine MOVEM performs movement calculations for each time step and calls subroutine MARKOV to determine the distributions of populations among habitats and soil layers. Subroutine APUM solves the toxicant mass balance equations by Runge-Kutta integration for the current concentrations of toxicant in the tissues of each animal group. APUM is called after all toxicant transport and animal movement calculations are completed for the current time step. Subroutine MDERIV is called by APUM to compute toxicant mass derivatives with respect to time; MDERIV also calls subroutines TOXASM, FEED, and PREDAT to estimate assimilation, feeding, and predation rates for each animal group. The pesticide intake rate for the population biomass is regulated using LD50, LD10 values in subroutine UPMOD.

The animal exposure submodel also includes several input, output, and general utility subroutines which are shown in hatched boxes in Figure 9.9. ANPRZM stores data needed by the submodel from PRZM transport calculations, including soil water contents and toxicant concentrations. Subroutine ANBAL performs mass balance calculations for the overall food chain and writes organism toxicant concentrations to output files at the end of each time step. These subroutines are called directly by the execution supervisor (EXESUP).

9.1.6 Monte Carlo Simulation

Monte Carlo simulation is performed by running the deterministic model a number of times with randomly selected inputs. The subroutines in module MCARLO facilitate this simulation. Of the subroutines shown in Figure 9.10, READM is called outside the Monte Carlo loop. This subroutine determines which TEEAM variables are specified by the user to be overwritten by randomly simulated variables and reads in their distribution parameters. Subroutine MCTRNS, called the first time outside the Monte Carlo loop overrides parameter values in the input files with the values of constants in the Monte Carlo input file. RANSET initializes the random number generators. INITMC eliminates constants in the Monte Carlo file from the

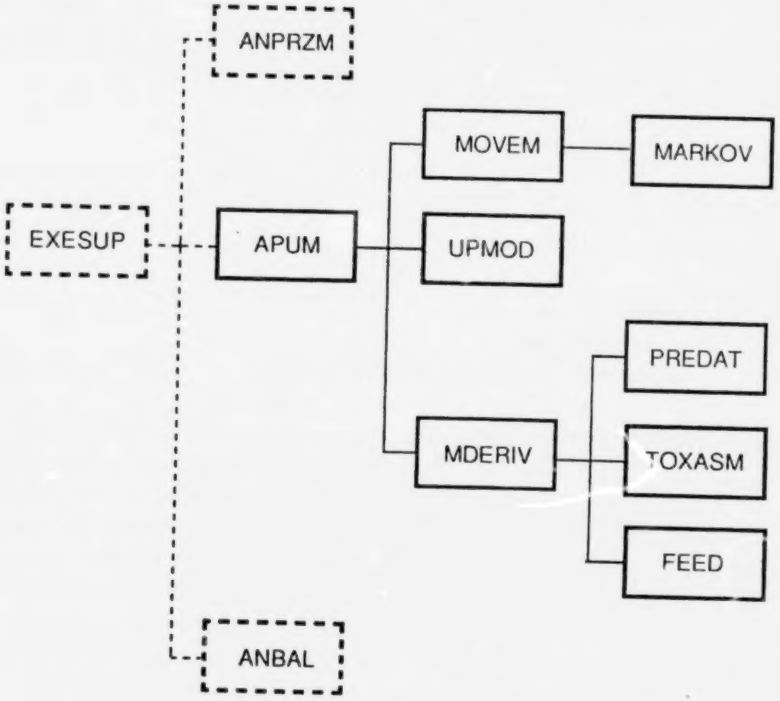


Figure 9.9 Module APUM structure.

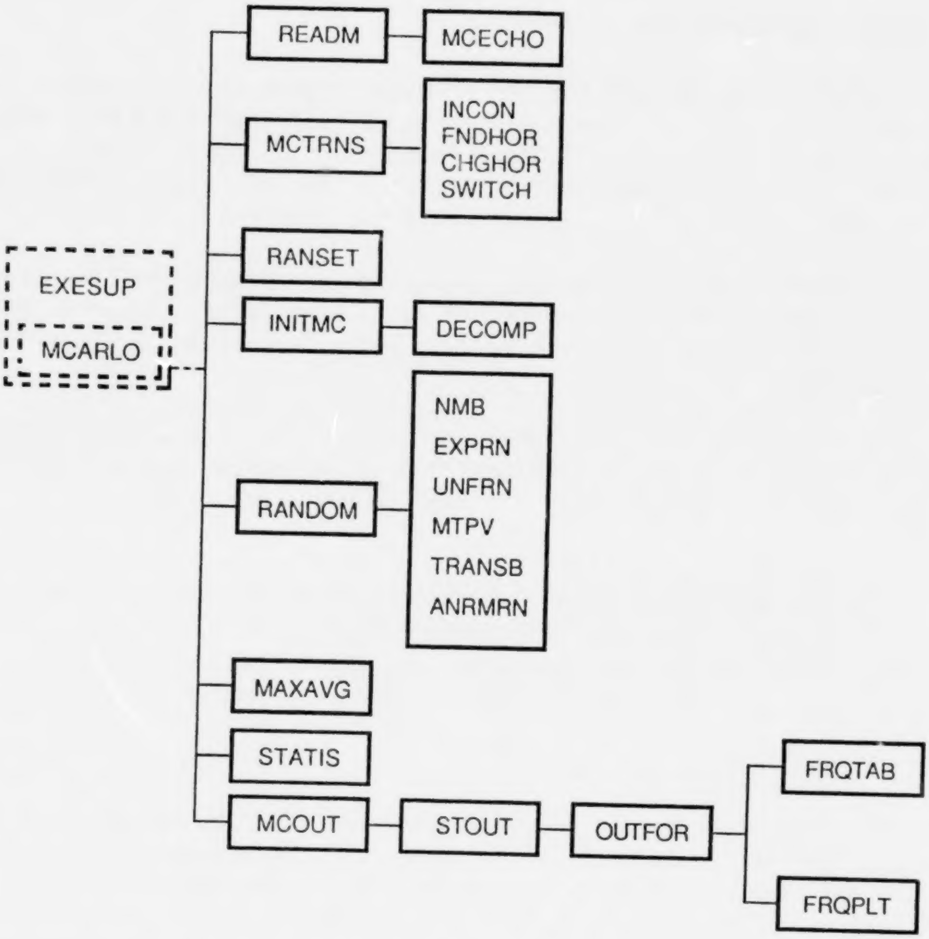

READM
MCECHO
MCTRNS
INCON
FNDHOR
CHGHOR
SWITCH
RANSET
EXESUP
MCARLO
INITMC
DECOMP
NMB
EXPRN
UNFRN
MTPV
TRANSB
ANRMRN
RANDOM
MAXAVG
STATIS
MCOUT
STOUT
OUTFOR
FRQTAB
FRQPLT

Figure 9.10 Module MCARLO structure.

list of Monte Carlo variables for the current run, conditions the correlation matrix and calls DECOMP to decompose the correlation matrix. Within the Monte Carlo loop, random variable values are generated by any of number of functions or subroutines called by RANDOM. MCTRNS then transfers these values to the proper variables in TEEAM. After the TEEAM time loops are complete, MCTRNS is called again to transfer the designated simulation output variables to the post-processor routines. MAXAVG finds the maximum values of an 'n' day moving average of the output time series. (The length of the averaging period 'n' is set by the user.) STATIS accumulates the statistics (sums, sums of squares, etc.) for the post-processors.

The Monte Carlo loop ends here. Once all Monte Carlo runs are complete, MCOUT is called to write output. STOUT computes means, moments, etc., of the output cumulative distribution functions (CDFs) and OUTFOR produces either tabular or printer plot summaries of the CDFs.

9.2 INTERMODULE COMMUNICATION

Data transfers occur through the use of named common blocks, subroutine arguments and scratch files. Common blocks normally contain data that are associated by topic, i.e., meteorological data are in a common block, hydrology data are in a separate common block. A list of common blocks and the topic of their contents is listed in Table 9-2 (see end of section).

Arrays in common blocks are variably dimensioned. Dimensions are given in PARAMETER statements which are contained in INCLUDE files. These INCLUDE files, their parameters and parameter default values are given in Table 9-3 (see end of section).

Subroutine arguments are used rather sparingly. They are primarily used to pass system level information or miscellaneous variables that are not in common. Occasionally, however, they are used to pass computational variables.

Scratch files are used to store major blocks of data, primarily for restarting simulations which have been temporarily suspended and transferring data between program modules. For more detailed descriptions of the use of scratch files, the user should read Section 9.4.

9.3 CODING CONVENTIONS

All of the modules contained in TEEAM were developed in, or upgraded to ANSI Standard FORTRAN 77 (X3.9-1978) language. The major transformation necessary in this conversion was to ensure that character data are stored in CHARACTER type variables. Some remnants of FORTRAN IV code may remain in the upgraded modules.

9.4 FILE UTILIZATION

This section discusses the use of files for program operation. Files required include input, output, and scratch files. Scratch files are useful in program operation for two reasons. First, by storing information in external files versus memory, memory requirements are reduced. This is important due to the size of the program and the memory limitations of PCs. Second, scratch files are used to facilitate the simulation of "multiple habitats." Simulation of multiple habitats involves the execution of the TFAT module, and other modules, several times within the same time loop iteration. Obviously, if not saved, the information generated from a TFAT execution would be overwritten when TFAT is next executed. Instead of saving all the information for each habitat in memory, it is written to external sequential files. While this results in lower memory utilization, it also slows program execution time.

The files utilized for the program are defined in Table 9-3, along with their default logical unit numbers. The utilization of the input and output files is self explanatory. The scratch files KHABS1 and KHABS2 are used in the following way. After the first habitat (TFAT module) is executed in timestep 1, the results are written to the KHABS1 file. Results for subsequent habitats are stacked sequentially in the KHABS1 file. At timestep 2, the initial conditions are read from the KHABS1 file and the results are written to the KHABS2 file. At timestep 3, the initial conditions are read from the KHABS2 file, results are written to the KHABS1 file and so forth. Thus, these files are read from or written to every other timestep. The HABIO subroutine, which reads and writes these files at each timestep, is also called after the initial parameter input read and initialization, to set up the unformatted initial conditions file for the first timestep.

Another file which is utilized in a unique way is the FSCBG output file (CBGDEP). On days when a spray application event occurs, the FSCBG program writes an output file which contains pesticide deposition information at each receptor point in the FSCBG grid. This file is read by subroutine GRDRD called from the TFAT module inside the habitat loop of the execution supervisor. For each habitat, the grid/habitat map overlay provided by the user is utilized to determine which grid points are within the habitat boundaries, and the area-weighted average deposition value for each habitat (see Figure 9.11). At the time of the next spray application event, the CBGDEP file is overwritten.

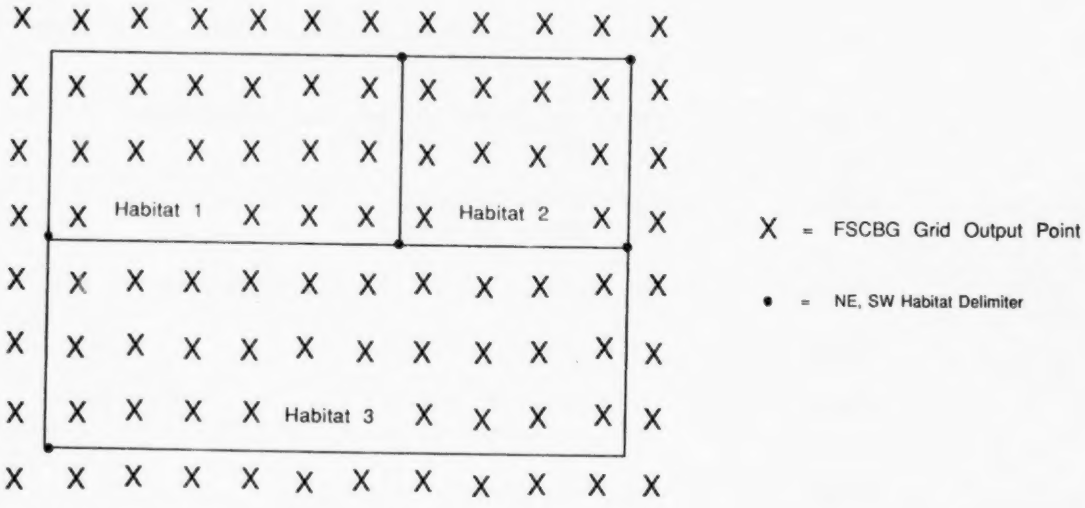


Figure 9.11 FSCBG linkage to TEEAM habitats.

Table 9-1. LIST OF SUBROUTINES BY MODULE AND DESCRIPTION OF THEIR FUNCTIONS

Module	Subroutine	Function
APUM	APUM	Solves for Changes in Pesticide Concentrations in Animals
	MDERIV	Computes Chemical Mass Derivatives for Each Animal Group
	TOXASM	Computes Mass Derivatives Due to Uptake From Fixed Media (i.e., soil, plants, air, ponded water)
	FEED	Computes Mass Derivatives Due to Feeding on Lower Trophic Levels
	PREDAT	Computes Mass Derivatives Due to Predation by Higher Trophic Levels
	ANBAL	Writes Pesticide Concentrations in Animals and Performs Mass Balances
	MOVEM	Computes Daily Animal Movement
	MARKOV	Computes Population Distribution Among Habitats or Soil Layers
	ANPRZM	Stores Data Needed by Animal Subroutine from Results of Each Habitat Simulation
	UPMOD	Modifies Uptake Rates to Account for Exceedance of Lethal Dosages
	INCON	Initializes Cumulative State Variables for Each Monte Carlo Run
FSCBG	CBGSO	Driver Routine for FSCBG Subroutine
	FSCBG	FSCBG Main Subroutine
	CBGS3	Calculates Parameters Used in Evaporation Model and Wake Settling Velocity
	CBGS4	Drop Evaporation Model
	CBGS6	Driver Routine for Dispersion Modules

Table 9-1. LIST OF SUBROUTINES BY MODULE AND DESCRIPTION OF THEIR FUNCTIONS (continued)

Module	Subroutine	Function
	CBGS7	Performs Dispersion or Dosage Calculations
	FSOUT	Prints Dispersion Model Calculations
	IOPUT	Prints Headings for Evaporation Model Input Data
	TRMVL	Calculates Terminal Velocities of Upper, Lower, and Average Drop Sizes Within a Category
	REGRS	Performs a Second Order Polynomical Regression
	(Function) SIMUL	Solves a Set of Simultaneous Linear Equations Using Gauss-Jordan Elimination With Full Pivoting
	TEST	Prints Actual and Predicted Values of Below Canopy Evaporation
	TESS	Performs Variable Assignments
	DROPD	Calculates Drop Diameters
	FOFX	Sets Standard Deviation Values and Decay Terms
	LNPN1	Sets up Parameter Values for Dosage and Deposition Model Solutions
	TITLR	Prints Table Headers
INITEM	INITEM	Determines User-Defined Options, Opens Files, and Reads Global Data
	GLBDAT	Initializes Global Data
	OPENF	Opens Files
	OPECHO	Printing Utility
	ELPSE	Printing Utility
	ECHOF	Echoes the Names of Files Opened
	CHKFIL	Checks to See Which Files Have Been Opened

Table 9-1. LIST OF SUBROUTINES AND DESCRIPTION OF THEIR FUNCTIONS (continued)

Module	Subroutine	Function
INPREA	INPREA	Driver Subroutine for Reading and Initializing Program Input Data
	PRZMRD	Reads and Checks TFAT (PRZM) Input Data
	PRZDAT	Initializes TFAT (PRZM) Data
	PZECHO	Echoes TFAT (PRZM) Data to an Output File
	PLTGRD	Reads and Checks Plant Growth Input Data
	PLECHO	Echoes Plant Growth Input Data
	HABIO	Reads and Writes Data to a Scratch File for Restarting Habitats
	SEQIO	Reads and Writes the Maximum Number of Records Possible to an Unformatted Scratch File
	CLOZE1	Closes One File
	APINIT	Initializes Animal Model Variables
	APUMRD	Reads, Checks, and Writes Animal Model Input Data
	PRDRED	Reads Animal Predation Data
	RANSET	Initializes the Random Number Generator
	INSTOR	Stores Initial Conditions for the Animal Model for Monte Carlo Simulation
	GRDDEF	Drives Subroutine for Reading and Printing Habitat/Receptor Grid Geometry
	GRDRD	Reads Habitat/Grid Receptor Geometry
	GRDOUT	Writes Habitat/Grid Receptor Geometry
	CKAREA	Checks the Error Between TFAT Input Habitat Areas and GRDDEF Calculated Habitat Areas
	CBGRD	Driver Subroutine to Read FSCBG Input Data (See also FSCDAT and FSRED2 described in Module TFAT)

Table 9-1. LIST OF SUBROUTINES AND DESCRIPTION OF THEIR FUNCTIONS (continued)

Module	Subroutine	Function
MCARLO	FSECHO	Echoes FSCBG Input Data
	ANRMRN	Generates Normally Distributed Random Numbers
	DECOMP	Decomposes Correlation Matrix into Coefficient Matrix Required to Generate Correlated Random Numbers
	EXPRN	Generates Exponentially Distributed Random Numbers
	FRQPLT	Writes Plots of Cumulative Frequency Distributions
	FRQTAB	Writes Tabulated Cumulative Frequency Distributions
	INITMC	Initializes Statistical Summation Arrays, Reorganizes Monte Carlo Input Arrays to Account for Constant Variables, and Performs Other Miscellenous Monte Carlo Initializations
	FNDHOR	Finds the Number of the First Layer in a Soil Horizon
	CHGHOR	Assigns a Parameter Value to All Layers in an Horizon
	SWITCH	Switches Monte Carlo Parameter Value for TEEAM Parameter Value
	MCECHO	Writes Monte Carlo Input Data to the Shell Output File
	MCTRNS	Transfers Values Between Monte Carlo Generated Arrays and TEEAM Variables
	MTPV	Multiplies a Vector of Uncorrelated Variables by a Coefficient Matrix to Form a Vector of Correlated Variables
	OUTFOR	Writes Frequency Tables and Plots
	OUTPUT	Writes Out Statistical Summaries of Monte Carlo Runs to the Monte Carlo Output File

Table 9-1. LIST OF SUBROUTINES AND DESCRIPTION OF THEIR FUNCTION (continued)

Module	Subroutine	Function
	RANDOM	Generates a Vector of Random Numbers From Specified Distributions
	READM	Reads Monte Carlo Input Data From a User-Specified Input File Unit Number
	STATIS	Performs Summations Required to Compute Statistical Moments for Random Model Inputs and Model Outputs Over All Monte Carlo Runs
	STOUT	Computes Statistical Moments (mean, standard deviation, skewness, kurtosis, correlations, minimum and maximum) From Summations Computed by STATIS. Statistics are then Written Out to the Monte Carlo Output File
	TRANSB	Transforms Normally Distributed Number to an SB Distributed Number
	TRANSM	Transforms Normally Distributed Numbers to Numbers Having the Appropriate User-Specified Distributions (i.e., log-normal, SB)
	UNFRN	Generates Uniform Random Numbers Ranging Between 0 and 1
	MCOUT	Writes Monte Carlo Summary Statistics
	MAXAVG	Computes Moving Average Values of Time Series Variables
	INCON	Restores Initial Conditions for APUM Module at the Beginning of a Monte Carlo Run
PLTGRN	PLTGRN	Driver Subroutine for Plant Growth Module
	DXGRO	Calculates Plant Growth Differentials
	PLTDAY	Calculates Daily Information for Plant Growth Simulation
	DAYLIT	Interpolates the Number of Daylight Hours on a Daily Basis From Monthly Data

Table 9-1. LIST OF SUBROUTINES AND DESCRIPTION OF THEIR FUNCTIONS (continued)

Module	Subroutine	Function
	PLTDEF	Retrieves Data for Current Plant From Storage Arrays
	INTERP	Linear Interpolation Routine
	SAVPLT	Writes Data for Current Plant Into Storage Arrays
	RK4GRO	Fourth-Order Runge-Kutta Routine to Solve Differential Plant Growth Equations
	PLTRNS	Driver Subroutine for Plant Translocation Module
PLTRNS	DEFTRN	Retrieves Translocation Data for Current Plant from Storage Arrays
	TRNDAY	Calculates Daily Information for Plant Translocation Simulation
	TRNDIF	Solves Differential Equations for Plant Translocation Using a Fully Implicit Scheme
	SAVTRN	Stores Translocation Information for the Current Plant into an Array
TFAT	TFAT	Driver Program for Terrestrial Fate and Transport Calculations
	PESTAP	Performs Chemical Application (not a spray event)
	PLGROW	Performs Plant Growth Calculations Per Original PRZM Code if PLTGRN is OFF or Calls PLTGRN
	PLPEST	Performs Fate and Transport Computations for Pesticides on Plant Foliage
	SLPEST	Sets Up Arrays for Tridiagonal Matrix Solution of Fate and Transport in Soil
	TRDIAG	Solves Tridiagonal Matrix Using the Thomas Algorithm
	EROSN	Performs Soil Erosion Calculations

Table 9-1. LIST OF SUBROUTINES AND DESCRIPTION OF THEIR FUNCTIONS (continued)

Module	Subroutine	Function
	EVPOTR	Computes Soil Evapotranspiration
	HYDR1	Performs Hydraulic Computations for Freely Draining Soils
	HYDR2	Performs Hydraulic Computations for Soils With Restricted Drainage
	MASBAL	Performs Water and Pesticide Mass Balance Computations
	HYDROL	Performs Surface Hydrologic Computations
	INFIL	Performs Infiltration Computations Using a Green-Ampt Model
	POND	Computes Depth of Surface Ponding
	PCHEM	Performs Chemical Fate Calculations for Surface Ponds
	VOLMT	Performs Computations for Pesticide Volatilization From Soil
	CANOPY	Computes Vegetative Canopy Resistance to Mass Transfer
	CNCONC	Computes Average Pesticide Concentration Within the Plant Canopy
	DEPMOD	Sets and Resets TFAT Pesticide Application Information When Spray (FSCBG) Events Occur
	GRANUL	Determines Chemical Release Rate from Granular Pesticides
SPECIO	METRD	Reads and Checks Meteorological Data
	RCHNUM	Computes Richardson Number from Meteorological Information
	GRDDEP	Driver Subroutine to Retrieve Deposition Data from FSCBG Output Files
	DEPRD	Reads FSCBG Output Deposition File

Table 9-1. LIST OF SUBROUTINES AND DESCRIPTION OF THEIR FUNCTIONS (continued)

Module	Subroutine	Function
	GRDAVE	Averages the Deposition Values in FSCBG Receptor Grid by Habitat and Computes Standard Deviation of Deposition Values
	AVEOUT	Writes GRDAVE Output
	FSCDAT	Data Initialization Routines for FSCBG
	FSRED2	FSCBG Input Data Reading Routine
	THCALC	Generates Water Content (Field Capacity/Wilting Point) from TFAT Input Data
	KDCALC	Calculates Pesticide Distribution Coefficient Values from TFAT Input Data
	OUTHYD	Writes Habitat Hydrologic Summaries
	OUTPST	Writes Habitat Pesticide Summaries
	OUTTSR	Writes Time Series Plotfile Data
	OUTCNC	Writes Habitat Pesticide Concentration Data
	INITL	Initializes TFAT Variables
UTIL	ERRCHK	Writes Error Messages, Closes Files if Fatal Error
	TRCLIN	Tracks Line of Program Being Executed
	LFTJUS	Left Justifies a Character String
	SCREEN	Screen Manager Routine
	CENTER	Centers a Character String
	DONBAR	Tracks the "Percentage Completeness" of the Program
	COMRD	Allows User to Insert Comments in Data Files by Ignoring Comments When Reading
	COMRDZ	Comment Reading Routine Which Handles End-of-File Read

Table 9-1. LIST OF SUBROUTINES AND DESCRIPTION OF THEIR FUNCTIONS (concluded)

Module	Subroutine	Function
	FILCHK	Checks "Open" Status of File
	ADDSTR	Adds a Character String to Another Character String
	NAMFIX	Left Justifies and Capitalizes a Character String
	BMPCHR	Capitalizes a Character String
	SUBIN	Routine Which Tracks Entry to Subroutines
	SUBOUT	Routine Which Tracks Exits From Subroutines
	EXPCHK	Test for Exponent Underflow/Overflow
	LOGCHK	Checks for Logarithm of a Negative Number
	ERFC	Complimentary Error Function
	ERF	Error Function
	RELTST	Converts Real Numbers From Double to Single Precision and Checks Overflow/Underflow

Table 9-2. COMMON BLOCK NAMES, TOPICS, AND INCLUDE FILE NAMES

Common Name	Topic Description	Include File Name
ANIM	Pesticide Uptake by Animals	CANM
ANIC	Label for Animal Model	CANM
CROP	Crop Growth and Pesticide Deposition	CCROP
ACCUM	Summary Output Accumulators for TFAT	CCUM
HYDR	Hydrology Information for TFAT	CHYDR
MET	Meteorological Information	CMET
MISC	Miscellaneous Variables (i.e., flags, etc.) for TFAT	CMISC
GLOBAL	Global Simulation Control Data (dates)	CMISC
CHMISC	TFAT Miscellaneous Titles, Output Control Data	CMISC
PEST	Pesticide Fate and Transport for TFAT	CPEST
PON	Ponding and Pond Chemistry Information	CPOND
CANOP	Pesticide Canopy Penetration Information	DQSCAN
FIXED	Pesticide Application Data (TFAT)	DOSGRN
DEPDAT	Information Required to Link FSCBG/TFAT	GRID
INITCM	Initial Conditions for Animal Exposure Module	INITCM
MOVE	Animal Movement Data	MOVE
MSBAL	Mass Balance Information for Animal Model	MSBAL
CMSBL	Labels for Animal Movement Model	MSBAL
PGCMP	Plant Growth Data	PGCMP
PGDAY	Daily Plant Growth Parameters	PGDAY
PGDEF	Plant Growth Data	PGDEF
PLANTS	Buffer for Plant Model Restart	PLANTS
PLFLUX	Plant Information to be Written Using Subroutine OUTPST	PLFLUX
RANDM	Used in Random Number Generator Initialization	RANDM
SPRAY	Canopy Penetration Data for Spray Application Events	SPRAY
TRACE	Subroutine Entry/Exit Data	TRACE
FSDAT	Spray Application Data	FSDAT

Table 9-3. PARAMETER STATEMENTS, PARAMETER DEFINITIONS, AND INCLUDE FILE NAMES

INCLUDE File Name	File Usage	Parameter	Default Value	Parameter Description
APARM	Animal Model	NL	5	Maximum Number of Predator Groups
		NH	4	Maximum Number of Habitats
		NS	5	Maximum Number of Soil Horizons
		NM	5	Maximum Number of Fixed Media (i.e., soil, water, plants, granules, seeds)
		NSG	3NH	Maximum Number of Soil Animal Groups
		NG	NL + NSG	Maximum Total Number of Animal Groups
		NTS	10	Maximum Number of APUM Time Series Plots
CMPLR.PAR	Compiler Specific	REALMX	1.0E23	Maximum Real Number
		REALMN	1.0E-23	Minimum Real Number
		MAXINT	2147483647	Maximum Integer
		MAXREC	512	Maximum Length of Unformatted File Record
		EXNMX	-53	Minimum Exponent
		EXPMX	53	Maximum Exponent
		EXPMN	REALMN	Maximum Result of Exponentiation
		PCASCI	TRUE	Logical Variable to Indicate if ANI.SYS is Present (if true, ANSI.SYS is present and machine is IBM PC compatible)
		CHR1WT	TRUE	Logical Variable to Indicate if Compiler Writes First Character in a String to the Screen (if true, character is written)
CPARM.PAR	TFAT Module	NCMPTS	33	Maximum Number of Soil Layers Plus 1
		NAPP	5	Maximum Number of Pesticide Applications
		NLVL	10	Maximum Number of Canopy Deposition Levels
		NC	5	Maximum Number of Crops

Table 9-3. PARAMETER STATEMENTS, PARAMETER DEFINITIONS AND INCLUDE FILE NAMES (continued)

INCLUDE File Name	File Usage	Parameter	Default Value	Parameter Description
GRID.PAR	FSCBG Receptor Grid	NH1	NH+1	Maximum Number of Habitats Plus 1
		NGRDSZ	25	Maximum Number of Grid Rows/Columns
		NGRDSQ	NGRDSZ^2	Number of Grid Rows/Columns Squared (i.e., Maximum Number of Grid Points)
HABIO	Scratch File Array Sizes for Restarting Habitats	NRLMIS	NCMPTS+18	Equivalence Arrays
		NI2MIS	NCMPTS+58	Equivalence Arrays
		NCHMIS	478	Equivalence Arrays
		NMIS	NI2MIS+2 (NRLMIS)	Equivalence Arrays
		NRLCRP	10+4(NC) +NLVL(NAPP) +2(NAPP)	Equivalence Arrays
		NI2CRP	8+9(NC) + NAPP	Equivalence Arrays
		NCRP	NI2CRP+ 2(NRLCRP)	Equivalence Arrays
		NRLPST	32+14(NCMPTS) +2(NAPP)	Equivalence Arrays
		NI2PST	3+2(NAPP)	Equivalence Arrays
		NDPPST	5(NCMPTS)	Equivalence Arrays
		NPST	NIZPST+ 2(NRLPST)+ 4(NDPPST)	Equivalence Arrays
		NRLHYD	22+15(NCMPTS) +3(NC)	Equivalence Arrays
		NI2HYD	8+10(NC)	Equivalence Arrays
		NHYD	NI2HYD+ 2(NRLHYD)	Equivalence Arrays

Table 9-3. PARAMETER STATEMENTS, PARAMETER DEFINITIONS AND INCLUDE FILE NAMES (continued)

INCLUDE File Name	File Usage	Parameter	Default Value	Parameter Description
		NRLCUM	76+20(NCMPTS)	Equivalence Arrays
		NCUM	2(NRLCUM)	Equivalence Arrays
		NRLPON	217	Equivalence Arrays
		NI4PON	1	Equivalence Arrays
		NPON	2(NRLPON + NI4PON)	Equivalence Arrays
		NRLPLT	NMPLNT (NSVAL + NPARAL)	Equivalence Arrays
		NPLT	2(NRLPLT)	Equivalence Arrays
IOUNIT.PAR	I/O Unit Defaults	KRUN	7	Unit No. for Run Parameters
		KPGDEF	11	Unit No. for Initial Conditions and Definition Parameters (Plant Growth)
		KPZDEF	13	Unit No. for Initial Conditions and Definition Parameters (PRZM)
	Input Files	KMCIN	15	Unit No. for Monte Carlo Data
		KPMET	9	Unit No. for Time Series (Meteorological) Data
		KAPIN	17	Unit No. for Animal Model Input
		GRDEF	19	Unit No. for Grid Definition
		CBGDEP	21	Unit No. for FSCBG Output
	Output Files	KUOUT	0	Unit No. for Output to User
		KECHO	8	Unit No. for Echo of Input Data
		KRSLTS	10	Unit No. for Animal Time Series
		KMCOUT	12	Unit No. for Monte Carlo Output
		KMCOU2	26	Unit No. for Monte Carlo Output
		KFLCN	14	Unit No. for Habitat Concentration Output
		KFLWT	16	Unit No. for Hydrology Output

Table 9-3. PARAMETER STATEMENTS, PARAMETER DEFINITIONS AND INCLUDE FILE NAMES (concluded)

INCLUDE File Name	File Usage	Parameter	Default Value	Parameter Description
		KFLPS	18	Unit No. for Habitat Pesticide Output
		KFLTS	20	Unit No. for Habitat Time Series Output
		KAPOUT	24	Unit No. for Animal Model Output
	Scratch Files	KHABS1	23	Unit No. for Multiple Habitat I/O
		KHABS2	25	Unit No. for Multiple Habitat I/O
		KMCINT	27	Unit No. for Monte Carlo Initial Conditions
		NMXFIL	20	Maximum Number of Files Which Can be Open
PLANTS.PAR	Plant Growth and Translocation	NMPLNT	10	Maximum Number of Plant Types
		NPARPG	10	Number of Parameters for Plant Growth
		NPARPT	6	Number of Parameters for Plant Translocation
		NPARAL	NPARPG +NPARPT	Total Number of Plant Growth Parameters
		NSVPG	10	Number of State Variables for Plant Growth
		NSVPT	2	Number of State Variables for Plant Translocation
		NSVAL	NSVPG +NSVPT	Total No. of Plant Translocation Parameters
PLTGRN.PAR		NEQN	9	Number of Differential Equations Solved for Plant Growth

SECTION 10

SIMPLE MODELS FOR PREDICTING TOXICANT ACCUMULATION IN TERRESTRIAL WILDLIFE: ATEEAM

10.1 MODEL DESCRIPTION

The Analytical Terrestrial Ecosystem Exposure Assessment Model (ATEEAM) code solves for pesticide concentrations in three components of a terrestrial foodchain; the soil, a soil dwelling organism and an upper trophic level predator. The system represented is shown in Figure 10.1. There are three variations on the system shown in the figure. These are designated models 1 through 3 and are described below. In all cases, the soil mass, animal biomass and rate constants are assumed to be constant. The equations are solved analytically which minimizes execution time. Solutions to the equations are given in Section 10.2. The code has an interactive preprocessor which allows the user to operate the model in either deterministic or Monte Carlo mode. This is discussed in Section 10.3.

10.1.1 Model 1. Single Toxicant Application with First-Order Soil Decay

Model 1 assumes that a single toxicant is applied to an agricultural field and undergoes first-order decay in the soil. The chemical is absorbed or otherwise taken up by a soil dwelling organism which can be in turn ingested by a higher trophic level predator (bird or small mammal).

The model for predicting pesticide concentration in the soil is

$$M_s \frac{dC_s}{dt} = - k_1 C_s M_s - k_2 C_s M_s - k_6 C_s M_s \qquad (10\text{-}1)$$

in which

M_s is the soil mass (kg)
C_s is the concentration of the toxicant in the soil ($\mu g\ kg^{-1}$)
k_1 is the first-order decay term for the toxicant in the soil (day^{-1})
k_2 is the first-order assimilation rate of pesticide (via absorption, ingestion or other processes) by the soil dwelling organism (day^{-1})

k_6 is the soil ingestion rate by the predator (day^{-1}).

This model assumes that the soil mass, M_s, does not change over time t. The model can be rewritten so that

$$\frac{dC_s}{dt} = -(k_1 + k_2 + k_6)\,C_s \qquad (10\text{-}2)$$

by dividing both sides through by the soil mass.

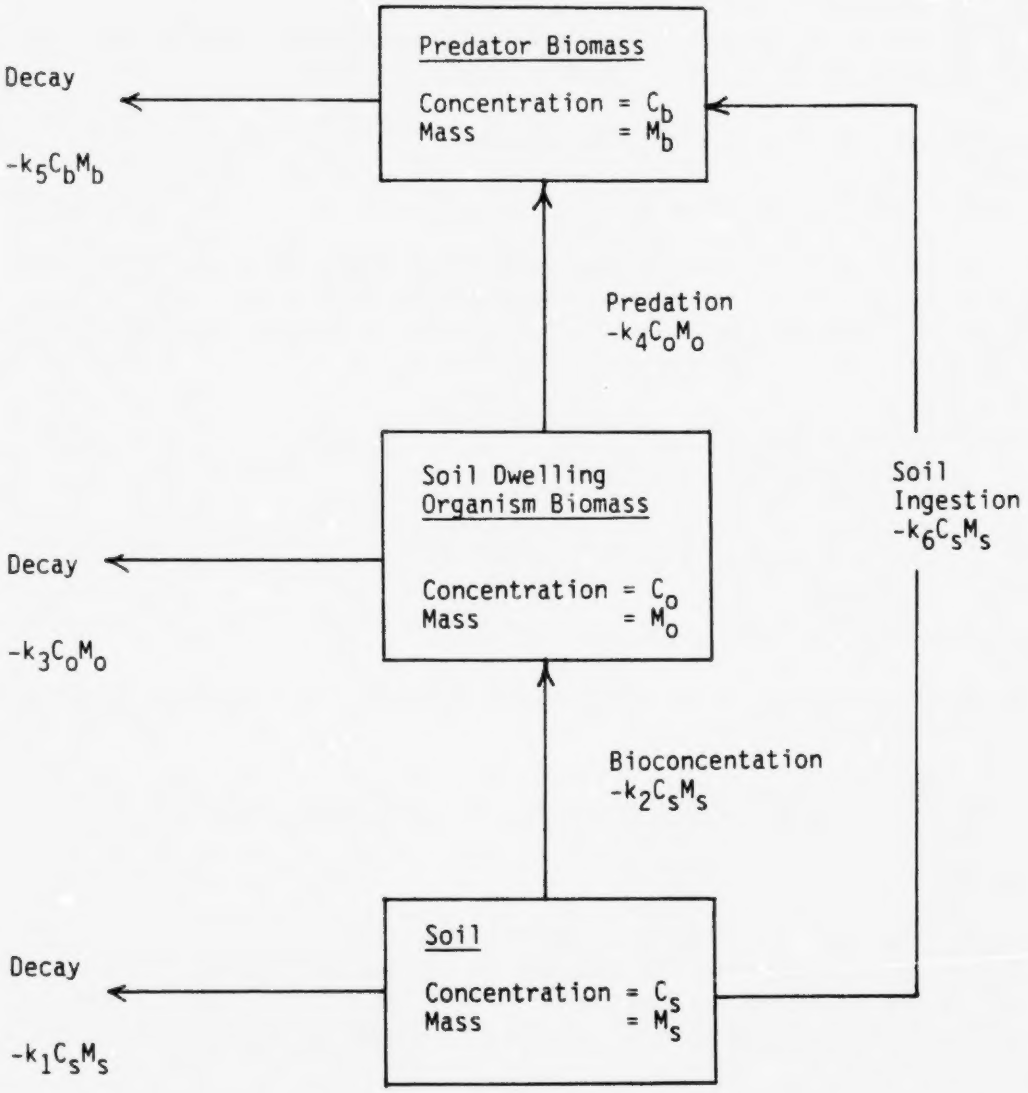

Predator Biomass
Concentration = C_b
Mass = M_b
Decay
$-k_5C_bM_b$
Predation
$-k_4C_oM_o$
Soil Dwelling Organism Biomass
Concentration = C_o
Mass = M_o
Decay
$-k_3C_oM_o$
Soil Ingestion
$-k_6C_sM_s$
Bioconcentation
$-k_2C_sM_s$
Soil
Concentration = C_s
Mass = M_s
Decay
$-k_1C_sM_s$

Figure 10.1. Schematic of A-TEAAM Model Structure

The contaminant mass balance equation for the soil dwelling organism is

$$M_o \frac{dC_o}{dt} = k_2C_sM_s - k_3C_oM_o - k_4C_oM_o \qquad (10\text{-}3)$$

in which

M_o is the biomass of the organism living in soil mass, M_s, (g)
C_o is the concentration of toxicant in the organism ($\mu g\ g^{-1}$)
k_3 is the first-order depuration rate of the toxicant by the soil dwelling organism (day^{-1}) (Note that the model assumes that any toxicant returned to the soil in this process is unavailable for reingestion, etc.)
k_4 is the predation rate by the higher level organism (day^{-1}) which is accumulated to the next trophic level

This equation can also be simplified to

$$\frac{dC_o}{dt} = \frac{k_2C_sM_s}{M_o} - (k_3 + k_4)\ C_o \qquad (10\text{-}4)$$

Note that this equation assumes that even though there is predation on the soil dwelling organism, the biomass remains at a steady level. A convenience is achieved also by dividing the first term on the right hand side by a unit volume (cm^3) of soil and defining

ρ_s as the soil bulk density ($kg\ m^{-3}$)
ρ_o as the organism density ($g\ m^{-2}$) and
Δz as the depth of soil involved (m)

Thus,

$$\frac{dC_o}{dt} = \frac{k_2C_s\rho_s\Delta z}{\rho_o} - (k_3 + k_4)\ C_o \qquad (10\text{-}5)$$

The mass balance equation for the predator (bird or small mammal) is given by

$$M_b \frac{dC_b}{dt} = k_4C_oM_o - k_5C_bM_b + k_6C_sM_s \qquad (10\text{-}6)$$

in which

M_b is the mass of the bird or small mammal (kg)
C_b is the concentration of toxicant in the tissue ($\mu g\ kg^{-1}$)
k_4 is the predation rate on the soil dwelling organism (day^{-1}) and
k_5 is the depuration rate of the bird or mammal of the toxicant (day^{-1})

The model assumes that the mass of the bird or small mammal stays constant over the simulation time 't'. The model is simplified by dividing through by the predator biomass giving

$$\frac{dC_b}{dt} = \frac{k_4 C_o M_o}{M_b} + \frac{k_6 C_s M_s}{M_b} - k_5 C_b \qquad (10\text{-}7)$$

Again, for convenience, the mass terms on the right hand side can be written in terms of densities, yielding

$$\frac{dC_b}{dt} = k_4 \frac{C_o \rho_o}{\rho_b} + k_6 \frac{C_s \rho_s \, \Delta Z}{\rho_b} \qquad (10\text{-}8)$$

in which

ρ_b is the biomass density of the predator over the area (A) of concern (kg A^{-1}). To be consistent with equation (10-5) A must be in m^2.

Also, for ease of parameter estimation the term $k_4 M_o$ can be thought of as a zero-order predation rate (g day^{-1}).

10.1.2 Model 2. Continuous Toxicant Application with First-Order Decay

Model 2 is the same as Model 1 which the exception of the description of toxicant accumulation in the soil. The equation for continuous application with first-order decay is

$$M_s \frac{dC_s}{dt} = L - k_1 C_s M_s - k_2 C_s M_s - k_6 C_s M_s \qquad (10\text{-}9)$$

where L is the application rate (μg day^{-1}) and all other terms are as defined previously.

10.1.3 Model 3. Steady-State Concentrations Under Continuous Deposition

The governing equations for the steady-state concentrations are simply found by setting the left hand sides of equations (10-9), (10-3), and (10-6) to zero.

10.2 SOLUTION OF MODEL EQUATIONS

The solutions to the system of ordinary differential equations which comprise models 1 and 2 are given below:

MODEL 1

Soil

$$C_s = C_s' e^{-at} \tag{10-10}$$

in which $a_1 = k_1 + k_2 + k_6$ and
C_s = the initial pesticide concentration in the soil.

Soil Dwelling Organism

$$C_o = C_o' e^{-bt} + \frac{k_2}{b - a} \frac{M_s}{M_o} C_s' (e^{-at} - e^{-bt}) \tag{10-11}$$

in which $b_1 = k_3 + k_4$ and
C_o = the initial pesticide concentration in the soil dwelling organism.

Predator

$$\begin{aligned} C_b &= C_b' e^{-k_5 t} \\ &+ \frac{M_s}{M_b} \left[\frac{k_2 k_4}{(b - a)(k_5 - a)} + \frac{k_6}{(k_5 - a)}\right] C_s' (e^{-at} - e^{-k_5 t}) \\ &+ \left[\frac{k_4}{k_5 - b} \frac{M_o}{M_b} C_o' + \frac{k_2 k_4}{(k_5 - b)(a - b)} \frac{M_s}{M_b} C_s'\right] (e^{-bt} - e^{-k_5 t}) \end{aligned} \tag{10-12}$$

in which C_b' is the initial pesticide concentration in the predator.

MODEL 2

Soil

$$C_s = \frac{L}{aM_s} (1 - e^{-at}) \tag{10-13}$$

in which $a = k_1 + k_2 + k_6$

Soil Dwelling Organism

$$C_o = \frac{k_2 L}{ab\, M_o} \left[1 + \frac{be^{-at} - ae^{-bt}}{a - b}\right] \tag{10-14}$$

in which $b = k_3 + k_4$

Predator

$$
\begin{aligned}
C_b = {} & \left(\frac{k_2\, k_4\, L}{k_5\, ab\, M_b} + \frac{k_6\, L}{k_5\, a\, M_b}\right)\left(1 - e^{-k_5 t}\right) \\
& + \left(\frac{k_2\, k_4\, L}{a(k_5 - a)\,(a - b)\, M_b} - \frac{k_6\, L}{a(k_5 - a)\, M_b}\right)\left(e^{-at} - e^{-k_5 t}\right) \\
& + \left(\frac{-k_2\, k_4\, L}{b(k_5 - b)\,(a - b)\, M_b}\right)\left(e^{-bt} - e^{-k_5 t}\right)
\end{aligned}
\tag{10-15}
$$

MODEL 3

Soil

$$C_s = \frac{L}{a\, M_s} \tag{10-16}$$

where $a = k_1 + k_2 + k_6$

Soil Dwelling Organisms

$$C_o = \frac{k_2 L}{ab\, M_o} \tag{10-17}$$

where $b = k_3 + k_4$

Predator

$$C_b = \frac{L}{M_b\, k_5}\left[\frac{k_4\, k_2}{ab} + \frac{k_6}{a}\right] \tag{10-18}$$

10.2.1 Solution Behavior

The solutions to the governing equations (e.g., equation 10-11) often have terms of the form

$$\frac{e^{-at} - e^{-bt}}{a - b} \tag{10-19}$$

which are indeterminant in the limit as a approaches b. The limit can be found using L'Hopitals Rule by which

$$\lim_{a \to b} \frac{e^{-at} - e^{-bt}}{a - b} = \frac{\frac{\partial}{\partial a}\left[e^{-at} - e^{-bt}\right]}{\frac{\partial}{\partial a}\left[a - b\right]} = -te^{-at} \tag{10-20}$$

Equation (10-20) shows that the limit exists and therefore that the solution in the limit is well behaved.

The practical consequence of this behavior is that the solutions provided give the exact solutions for all cases except when a identically equals b. Such a condition is of no interest practically as there is no a priori reason why the sum of the rate constants represented by a and b would be equal. If for some reason the user would like to examine such a case, the value of either a or b should be perturbed by a small amount (perhaps one percent).

10.3 MODEL ACQUISITION, INSTALLATION, AND EXECUTION

The ATEEAM model is available on 5-1/4-inch floppy diskettes for MS-DOS compatible computers. The model can be obtained by contacting Dr. David S. Brown at the EPA's Athens Georgia Environmental Research Laboratory (US EPA, Environmental Research Laboratory, Assessment Branch, College Station Road, Athens, GA 30613).

The model diskette contains the model FORTRAN code (source and executable) and sample input and output files. A listing of the files contained on the disk is given below.

ANIMAL.FOR	ATEEAM FORTRAN code
ANIMAL.EXE	ATEEAM executable code
DECAY.INC	Common blocks containing pesticide decay and uptake rates. This file is INCLUDED in ANIMAL.FOR during compilation.
MCARLO.INC	Common blocks containing the system descriptive data. It is INCLUDED in ANIMAL.FOR during compilation.
MODEL1.INC	Common blocks containing the model control parameters. It is INCLUDED in ANIMAL.FOR during compilation.
PARAM.INC	Parameter statements defining the size of arrays dimensioned in ANIMAL.FOR. It is INCLUDED in ANIMAL.FOR during compilation
SAMPLE.IN	Sample input file for batch mode operation.

SAMPLEB.OUT	Sample output file produced when running in batch mode using SAMPLE.IN
SAMPLEI.OUT	Sample output file produced when running in interactive mode using default values.

10.3.1 Hardware

To run the ATEEAM model an IBM PC, XT or AT compatible computer with one floppy disk drive is required. A hard drive is not required but is advisable. If running without a hard disk the floppy disk receiving the model output must have enough storage remaining to contain all of the output. When running in Monte Carlo mode this output can be considerable, depending upon the number of Monte Carlo runs and the number of variables randomly generated. At a minimum, the main output file requires 90 Kbytes of storage.

The executable file (ANIMAL.EXE) included with the model requires a math coprocessor chip, either an INTEL 8087 or 80287. If one is unavailable the source code can be recompiled using a compiler which does not require a coprocessor.

10.3.2 Software

The only software required to run the ATEEAM model, besides an executable version of the model, are:

- * DOS
- * ANSI.SYS

The ANSI.SYS device driver is included with DOS. This driver is installed by inserting the command:

```
DEVICE = ANSI.SYS
```

in the CONFIG.SYS file. If the CONFIG.SYS file does not exist it can be created using either a text editor or word processor or the DOS copy command. The user should consult a DOS manual if more information is needed.

10.3.3 Installation and Execution Instructions

If a hard drive is available, copy the model from the diskette to the hard drive. It is best if the model is kept in its own directory on the hard drive. In order to create a directory, after booting the computer type:

```
MD ANIMAL
CD ANIMAL
```

To copy the model onto the hard disk, insert the floppy into the A: drive and type:

```
COPY A:*.*
```

If a hard drive is not available, make a copy of the diskette containing the model. Save the original and use the copy. To run the model, insert the copy of the model diskette into the A: drive.

To run the model for either case discussed above, type:

```
ANIMAL
```

A title screen will appear and the user will be prompted for information to run the model.

10.4 MODEL INPUT SEQUENCE DEVELOPMENT

This section discusses the development of batch input sequence and interactive model operation.

Each of the model parameters are assigned default values in the model. Tables 10.1 and 10.2 list these values. If the user wishes to run the model with a different set of parameters there are two methods available to change these values, either by reading new values from a file (batch mode) or by changing them interactively. A discussion of the formats required for the batch mode and a sample run through the interactive mode follows the description of the input parameters.

10.4.1 Input Parameter Description

There are two basic types of input data, Simulation Control Parameters, and System Descriptive Parameters.

There are 12 simulation control parameters. These 12 variables are listed below along with a short description of each.

NMCR	Number of Monte Carlo simulations to perform.

NCAT	Number of periods to divide the output into. The length of these periods are defined by the user. (see Section 10.7 for more details).
THRSHO	Lethal whole body concentration for the lower trophic level animal. This value corresponds to a concentration such as an LC50 (tissue concentration). It is only used for comparison to whole body concentration generated by the model.
THRSHB	Lethal whole body concentration for the higher trophic level animal. This value corresponds to a concentration such as an LC50 (tissue concentration). It is only used for comparison to whole body concentration generated by the model.
DOSAG1	Lethal dosage for the lower trophic level animal. It is used for comparison with model output dosages. It corresponds to a value such as the LD50.
DOSAG2	Lethal dosage for the higher trophic level animal. It is used for comparison with the model output dosages. It corresponds to a value such as the LD50.
Starting and Ending Dates	These six control parameters are the starting and ending day, month and year of the simulation.

The simulation period can be divided into a number of intervals or periods for output. Dates corresponding to the end of each period except for the last are input. The last period ends on the last day of the simulation. This results in NCAT - 1 periods.

System descriptive parameters are those which appear in the model equations. In general, these parameters are defined by name, mean, coefficient of variation, minimum and maximum allowed values and distribution type. If a distribution is defined for a parameter the value

TABLE 10.1. DEFAULT VALUES FOR ATEEAM MODEL CONTROL PARAMETERS

VARIABLE NAME	DEFAULT VALUES
NMCR	100
NCAT	3
NP	6
THRSHO	20
THRSHB	4000
DOSAG1	45
DOSAG2	65
MODEL1	SINGLE APPLICATION

of the parameter used by the model is randomly generated based upon the distribution type and distribution parameters. If the distribution type is constant then the parameter takes the mean value. If all of the parameters are input as a constant then the model defaults to a deterministic mode. More details on the differences between Monte Carlo mode and deterministic mode are given in Section 10.6. Below is a list of the parameter names which corresponds to designations used in Sections 10.1 and 10.2.

PARAMETER NAME	PARAMETER DESIGNATION (corresponding to Equations in Section 10.1)
DECAY1	k_1
RATE12	k_2
DECAY2	k_3
RATE23	k_4
DECAY3	k_5
RATE13	k_6
MASS1	M_s
MASS2	M_o
MASS3	M_b
CONC1	C_s
CONC2	C_o
CONC3	C_b

When inputting data, keep the following points in mind. Only the last two digits of the year are necessary. The coefficient of variation is in percent; therefore, it is equal to the mean divided by the standard deviation times 100. The mean has to be between the minimum and maximum values. If it is outside these bounds the run stops and an error message is written to the output file. The distribution type is an integer indicating the type of distribution required. The choices are:

TABLE 10.2. DEFAULT VALUES FOR SYSTEM DESCRIPTIVE PARAMETERS[a]

VARIABLE NAME	MEAN	COEFF. OF VARIATION	MINIMUM	MAXIMUM	DIST.
DECAY1	0.02	100	0.00	10.0	NORMAL
RATE12	6.7E-06	50	0.00	1.0E-03	NORMAL
DECAY2	0.02	100	0.00	0.10	NORMAL
RATE23	1.02E-04	50	0.00	5.0E-03	NORMAL
DECAY3	1.20	100	0.00	5.0	NORMAL
RATE13	2.15E-10	100	0.00	1.0E-05	NORMAL
MASS1	5.63E+08	10.0	0.00	0.27E+11	NORMAL
MASS2	3.75E+04	10.0	0.1	3.0E+06	NORMAL
MASS3	80.0	10.0	0.1	8000	CONSTANT
CONC1	7.50	10.0	0.1	10.0	CONSTANT
CONC2	0.0	0.0	0.0	1.0	CONSTANT
CONC3	0.0	0.0	0.0	1.0	CONSTANT

---

[a] Units of all decay/transfer rates are day^{-1}; mass, g; concentration µg g^{-1}.

DIST	DISTRIBUTION
0	CONSTANT
1	NORMAL
2	LOGNORMAL

When simulations are run in Monte Carlo mode the user has the option of specifing correlations between descriptive parameters. However, the model can generate correlated parameters only when the correlated parameters are defined using normal distributions. The user must be careful when specifing correlations between variables having lognormal distributions. Parameters with lognormal distributions can be correlated with other parameters having normal or lognormal distributions if the correlation coefficient between the parameters is between values in normal space. For example, if DECAY3 and RATE13 were specified by the user as lognormally distributed random numbers with a correlation coefficient of 0.9, the model would generate two normally distributed random numbers with a correlation coefficient of 0.9 then transform these results using a lognormal transformation. Of course, parameters specified as constants will have no correlation with other parameters even though such a relationship is specified.

Lastly, the user must specify a seed for the random number generator. This number must be an integer between 1 and 2147483647. It is used to initialize the generator. A given seed will produce a unique sequence of random numbers. Different seeds produce different sequences of random numbers with the same distribution statistics.

10.4.2 Batch Input Sequence

The formats shown in Table 10.3 are used to enter the above data using a batch input file. The control data has to be input in the order specified. The system descriptive parameters can be input in any order. For the descriptive data, the model associates the data with the name read in, not with the order in which it is read. Besides data, the data file can also contain comments. These are identified by the presence of three stars ('***') as the first three non-blank characters on a line.

The descriptive parameter data must be followed by a data line containing the word END. This can be anywhere on the line but must be the first three non-blank characters. This indicates that there are no more descriptive parameters to read in. For the balance of the required parameters, the model will use default values. The same is true for the correlation data. There must also be an END after the last correlation data set. This indicates the end of the data file.

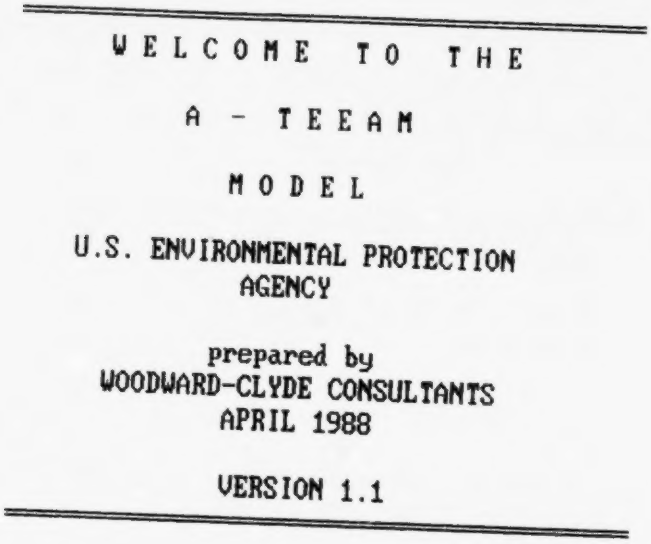
TABLE 10.3. FORMATS FOR BATCH INPUT FILE

FORTRAN NAME	DESCRIPTION OF INPUT	UNITS	DATA FORMATS
TITLE	Title of run	NA	A80
NMCR,NCAT	Number of simulations, Number of output periods	NA	2I5
DAY,MONTH,YEAR	Starting date of the simulation	NA	3I5
DAY,MONTH,YEAR	Ending date of the simulation	NA	3I5
THRSHB,THRSHO, DOSAG1,DOSAG2	Concentrations and dosages used for output comparison	ug/g ug	4F8.0
LOAD	Loading data if using continuous application model (else omit)	ug/day	F8.0
NAME,MEAN,COEF. VAR., MIN, MAX, DIST	Name, mean of distribution, Coefficient of Variation, Minimum and Maximum of distribution and distribution type	NA, 1/day, %, 1/day, 1/day, NA	A8, 2X, 4G10.4, 2I5,
END	Data line indicating end of descriptive data	NA	A3
NAME1, NAME2, CORR	Correlation coefficient data	NA	2(A8,2X), F10.0

10.4.3 Interactive Input

The interactive input is largely self explanatory, but a brief description of each screen follows.

The first screen after the title screen (screen 1, Figure 10.2) asks for the name of the output file (screen 2, Figure 10.3). It is assumed that this is a new file. If the file already exists, (screen 3, Figure 10.3) will appear and ask if it is permissible to overwrite the file or to stop the program. To overwrite type the letter O. To stop the program type the letter S. If the option to overwrite is chosen, output



```
WELCOME TO THE

A - TEEAM

MODEL

U.S. ENVIRONMENTAL PROTECTION
AGENCY

prepared by
WOODWARD-CLYDE CONSULTANTS
APRIL 1988

VERSION 1.1
```

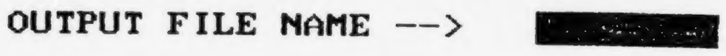
```
-- HIT RETURN KEY WHEN READY --
```

Figure 10.2. Screen 1 ATEEAM model title screen

from previous runs which used the same output file name may be lost. The model creates output files which contain results from either the Monte Carlo simulations or the time series results from deterministic simulations, (see Section 10.6 for description of output files). If these files already exist, screen 4 (Figure 10.3) appears and the same procedure as above should be followed.

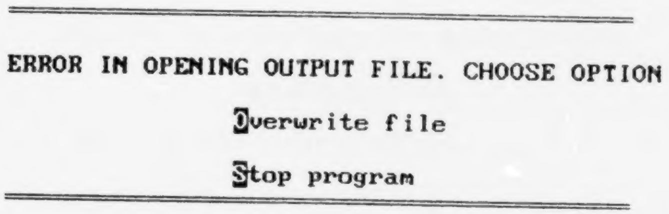
Screen 5 (Figure 10.4) gives the user an option as to which model to run. The response should be a 1, 2 or 3. A description of each model is given in Section 10.1. The next screen (screen 6, Figure 10.4) offers the choice of running the model in batch or interactive mode. If batch mode is desired, type the letter B. The user will then be asked for the name of the input file and the random number generator seed. If interactive mode is desired type the letter I. The user will be prompted for additional data by additional screens.

Model control parameters are input next (screen 7, Figure 10.5). The default values for the parameters will appear on the screen. The default values will initially appear in reverse video but will convert to normal



```
OUTPUT FILE NAME -->
```

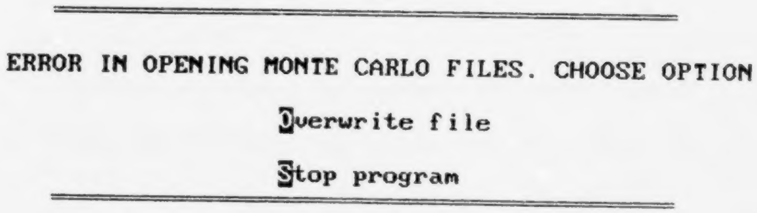
Screen 2. Request for output file name



```
ERROR IN OPENING OUTPUT FILE. CHOOSE OPTION
                Overwrite file
                Stop program
```

Screen 3. Error indicated in opening output file. Possible responses:

O - Overwrite existing file
S - Stop program execution



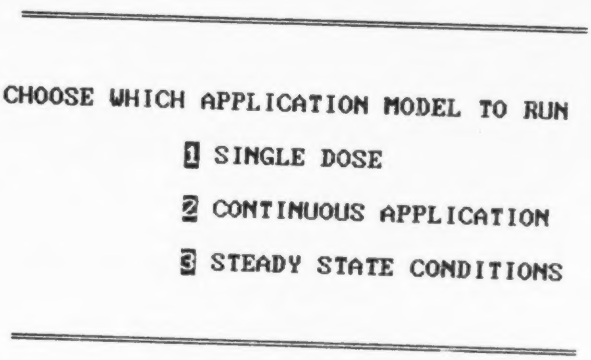
```
ERROR IN OPENING MONTE CARLO FILES. CHOOSE OPTION
                  Overwrite file
                  Stop program
```

Screen 4. Error indicated in opening model output files. Possible responses:

O - Overwrite existing files
S - Stop program execution

Figure 10.3. Screens 2, 3 and 4 from ATEEAM model

video when a value is input. For each parameter either the default value can be retained or a new value can be assigned. The value presently assigned to each parameter will appear in the lower right hand corner of the screen. Entering a carriage return will retain this value and advance the cursor. If a new value is desired, type in the number and a carriage return. When a carriage return is entered after the last number the cursor returns to the top of the screen to give the user a chance to correct any mistakes or change more values. When everything on the screen is correct, the user should input a Q and a carriage return. This will end input for the control parameters.



```
CHOOSE WHICH APPLICATION MODEL TO RUN

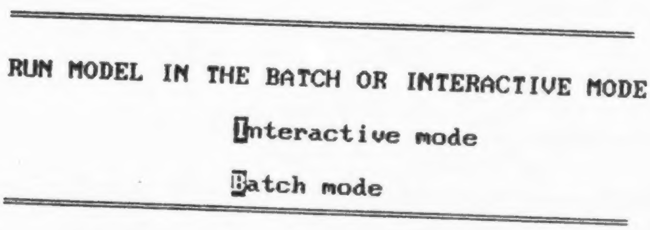
        1 SINGLE DOSE

        2 CONTINUOUS APPLICATION

        3 STEADY STATE CONDITIONS
```

Screen 5. Indicate type of simulation to run. Possible responses:

1 - Simulation of single application of pesticide
2 - Simulation of continuous application of pesticide
3 - Simulation of steady-state conditions (continuous application)



```
RUN MODEL IN THE BATCH OR INTERACTIVE MODE

        Interactive mode

        Batch mode
```

Screen 6. Indicate if input is in batch or interactive mode. Possible responses:

I - Interactive mode
B - Batch mode

Figure 10.4. Screens 5 and 6 from ATEEAM model

If more than one output period is requested (NCAT > 1) then screen 8 (Figure 10.5) will appear requesting the ending dates for each period except the last. (The last period is assumed to end on the last day of the simulation.) The ending day, month (1 - 12) and the last two digits of the year are input. The user will continue to be prompted for input until all the necessary data are entered. If after entering a carriage return the cursor doesn't advance, there is an error in input. The error could be something such as a month greater than 12, too many days in a month or the periods out of chronological order. After the last date has been entered, the cursor will go back to the top of the screen. At this point the user can either re-enter the data, if there was a mistake for example, or enter a Q. Entering a Q will bring up the next screen.

Screen 9 (Figure 10.6) contains the descriptive parameters. As was the case for the control data, default values are assigned to these variables and they will appear on the screen. If the default data is acceptable, enter a carriage return and the cursor will move to the next data point. If a different value is desired, type it and enter a carriage return. By using the 'U' and 'D' keys, the user can move up or down on the screen entering only selected data points. Typing 'D' and return will move the cursor to the beginning of the next line down. Typing 'U' and return will move the cursor to the beginning of the previous line. When all the data is satisfactorily entered the user types Q and carriage return.

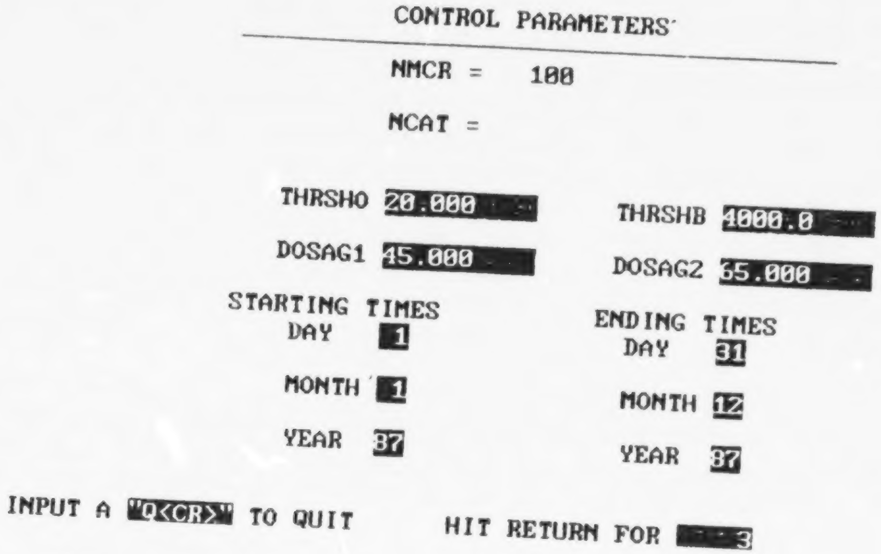
The last screen (screen 10, Figure 10.6) allows the user to input parameter correlation information. There are three pieces of data necessary for each correlation. The user has to input the names of the two correlated parameters (DECAY1, RATE12, etc....) and the correlation coefficient between them. The correlation coefficients must be between -1 and +1 and follow the limitations specified in Section 10.4.1. Hitting a carriage return without inputting any data on a line will signify the end of data input for this screen.

After completing all of the above screens the last question asks the user to input an integer used as the seed to the random number generator. This number can be any integer between 1 and 2147483647.

10.5 PARAMETER ESTIMATION

There are 12 parameters which must be given values in order to operate the ATEEAM code. These parameters break down into three groups:

- Mass estimates
- Rate constants
- Initial pesticide concentrations in biomass



```
                    CONTROL PARAMETERS
                NMCR =    100

                NCAT =

         THRSHO 20.000               THRSHB 4000.0

         DOSAG1 45.000               DOSAG2 35.000

       STARTING TIMES              ENDING TIMES
         DAY    1                    DAY    31

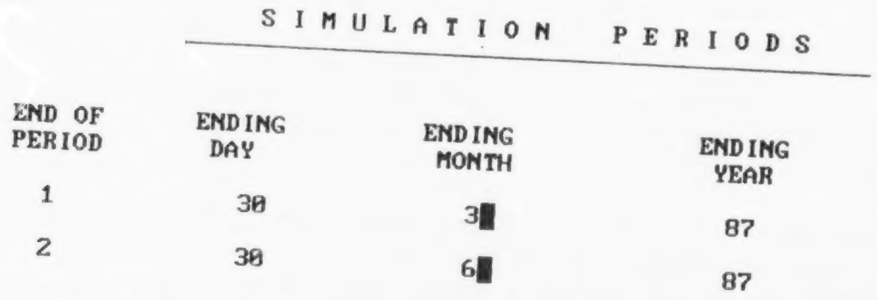
         MONTH  1                    MONTH  12

         YEAR   87                   YEAR   87

INPUT A "Q<CR>" TO QUIT         HIT RETURN FOR    3
```

Screen 7. Input model control data. Possible responses:

Value - New value to assign to parameter
"CR" - Retain present value of parameter that is indicated in lower right hand corner of screen
Q - Finished model control parameters. Go to next screen



```
           S I M U L A T I O N   P E R I O D S

END OF       ENDING        ENDING          ENDING
PERIOD       DAY           MONTH           YEAR

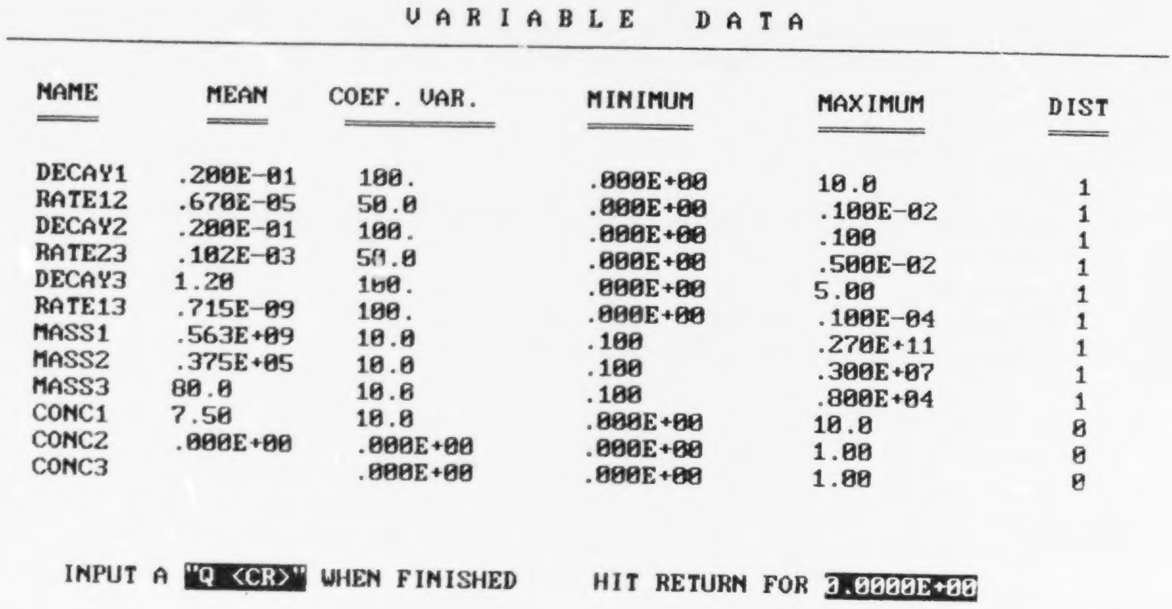
  1            30            3               87

  2            30            6               87
```

Screen 8. Input ending dates of each output period. Possible responses:

Date - Ending day, ending month and ending year of period
Q - Finished simulation period data. Go to next screen

Figure 10.5. Screens 7 and 8 from ATEEAM model running in interactive mode



```
                     V A R I A B L E   D A T A
 ____________________________________________________________________

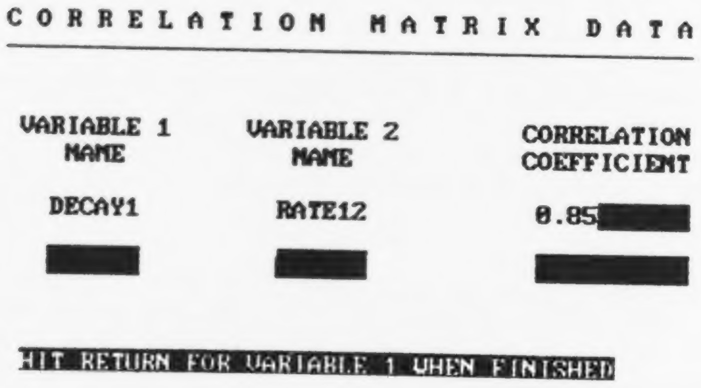
 NAME      MEAN      COEF. VAR.      MINIMUM       MAXIMUM       DIST
 ====      ====      ==========      =======       =======       ====

 DECAY1   .200E-01   100.           .000E+00      10.0            1
 RATE12   .670E-05   50.0           .000E+00      .100E-02        1
 DECAY2   .200E-01   100.           .000E+00      .100            1
 RATE23   .102E-03   50.0           .000E+00      .500E-02        1
 DECAY3   1.20       100.           .000E+00      5.00            1
 RATE13   .715E-09   100.           .000E+00      .100E-04        1
 MASS1    .563E+09   10.0           .100          .270E+11        1
 MASS2    .375E+05   10.0           .100          .300E+07        1
 MASS3    80.0       10.0           .100          .800E+04        1
 CONC1    7.50       10.0           .000E+00      10.0            0
 CONC2    .000E+00   .000E+00       .000E+00      1.00            0
 CONC3               .000E+00       .000E+00      1.00            0


   INPUT A "Q <CR>" WHEN FINISHED      HIT RETURN FOR 0.0000E+00
```

Screen 9. Input screen for system descriptive parameters. Possible responses:

Value - New value to assign to parameter
"CR" - Retain present value of parameter that is indicated in lower right hand corner of screen
"U" - Move the cursor to the beginning of the previous line
"D" - Move the cursor to the beginning of the next line
"Q" - Finished descriptive parameter input. Go to next screen



```
 C O R R E L A T I O N   M A T R I X   D A T A
 _____________________________________________

 VARIABLE 1     VARIABLE 2      CORRELATION
    NAME           NAME         COEFFICIENT

  DECAY1         RATE12          0.85


 HIT RETURN FOR VARIABLE 1 WHEN FINISHED
```

Screen 10. Input screen for correlation data. Possible responses:

Parameter Name - Enter the names of the two parameters which are correlated
Correlation Coefficient -
Q - Finished

Figure 10.6. Screens 9 and 10 from running ATEEAM model in interactive mode

Each of these categories of parameters is discussed in the following sections. Special considerations for estimating parameters required for Monte Carlo analysis are covered last.

10.5.1 Mass Estimates

There are three masses which must be estimated as input to the model:

- Soil mass
- Lower trophic level (soil dwelling organism) population biomass
- Upper trophic level (predator) biomass

10.5.1.1 Predator Biomass--

The easiest way to define the system is by beginning with an estimate of the areal extent of the habitat for a single predator. For example, if the predator is the passerine bird T. migratorius, then the habitat or territory is approximately 0.15 ha. The biomass of an adult robin living in this 0.15 ha is approximately 80 grams; therefore, M_b the biomass of the predator would be 80 grams.

10.5.1.2 Soil Dwelling Organism Biomass--

The estimation of the biomass of the soil dwelling organism is straightforward once the habitat size is known. Normally, the density of organisms is defined in terms of number or biomass per unit area (usually m^2). To obtain the biomass, one simply takes the product of the habitat area and the biomass density (e.g., g m^{-2}). If the number instead of biomass per unit area is given, then the average weight of an individual of the species must also be known in order to obtain the biomass. Typical biomass densities for a number of soil dwelling organisms was given in the parameter estimation section (Section 6.7.1) of the TEEAM documentation. As an example, for cropland, Lee (1985) provided estimates of 0.5 to 20 g m^{-2} for earthworms. If the size of the habitat is 0.15 ha and the biomass density of 20 g m^{-2} is used, then the biomass M_o is 30,000 grams.

10.5.1.3 Soil Mass--

The mass of the soil is easily estimated by taking the product of the soil bulk density (g cm^{-3}) with the habitat area (ha) and a representative depth of soil (cm). Bulk densities for various soil types were given in Section 6 (Table 6-26). The main problem in producing this mass estimate is choosing a representative soil depth. By choosing a depth that is too large, concentrations of the chemical in soil may be underestimated, and conversely, if the depth is too small they may be overestimated. The depth used should ideally be the depth to which the chemical is mixed over the period of the simulation. This might be a function of the depth of activity of soil dwelling animals, or the depth of movement of the bulk of the chemical mass (by leaching) over the period of the simulation. The latter can be estimated by assuming plug flow and using

$$D = \frac{RV\Delta t}{\Theta} \qquad (10\text{-}21)$$

in which D is the depth of movement (cm)
R is the chemical retardation factor (dimensionless)
V is the average recharge rate over the period and
Δt (cm Δt^{-1}) and
Θ is the average water content of the soil over Δt (cm^3 cm^{-3})

The retardation factor is calculated by

$$R = 1 + \frac{K_{oc}(OC)_{\rho s}}{\Theta} \qquad (10\text{-}22)$$

in which

K_{oc} is the organic carbon partition coefficient for the chemical (cm^3 g^{-1})

OC is the soil organic carbon content (fraction, g g^{-1})

ρ is the soil bulk density (gcm^{-3})

However, since the highest exposures are likely to occur immediately after application, the user may wish to bias such a calculation towards shallower depths. For convenience, in this discussion, a depth of 15 cm is utilized. This is a typical "plow layer depth" in agricultural soils and a depth to which the chemical might be readily mixed by bioturbation in a relatively short time. Using 15 cm as the representative depth, and a bulk density of 1.5 g cm^{-3}, the soil mass in 0.15 ha would be 3.4 x 10^8 grams.

10.5.2 Rate Constants

In this model, six rate constants can be utilized:

- k_1 is the degradation rate of the chemical in soil
- k_2 is the transfer rate of the chemical from the soil to the lower organism biomass
- k_3 is the clearance rate of the chemical from the lower organism biomass
- k_4 is the transfer rate from the lower organism to the predator
- k_5 is the clearance rate of the chemical from the predator and
- k_6 is the transfer rate from the soil directly to the predator.

10.5.2.1 Degradation Rate in Soil--

The user should refer to Tables 6-20 and 6-21 provided in Section 6. If information for the chemical of interest is not available, then registrant data or other sources of information may be used. The degradation rate must be entered in day^{-1}.

10.5.2.2 Transfer Rates--

Three of the rate constants, k_2, k_4, and k_6, deal with transfers, related primarily to ingestion, between mass compartments. Transfer from the soil to the soil dwelling organism may be accomplished through ingestion or by dermal absorption. Ingestion rates for soil and plant litter for various soil dwelling organisms may be found in Section 6.7.3.1. These are normally given in grams of soil per gram of organism body weight per day. To obtain the rate constant, simply take the product of this rate and the organism biomass, M_o, and divide by the soil mass M_s. For example, in the case of earthworms, a typical soil ingestion rate is 0.08 g g^{-1} day^{-1}. Therefore a typical value for the rate constant k_2 would be

$$k_2 = \frac{0.08\ (30{,}000\ \text{grams})}{3.4 \times 10^8\ \text{grams}} = 7.1 \times 10^{-6}\ \text{day}^{-1}$$

Similarly, the ingestion rate of earthworms by avian predators is typically given in g g^{-1} day^{-1} (or perhaps another time unit). Or the user may have information on total food intake and food preferences (%) in which case, the product of the two will give the ingestion rate for the prey. A typical ingestion earthworm rate for T. migratorius would be 0.1 g g^{-1} day^{-1}. Therefore the rate constant k_4 is

$$k_4 = \frac{0.06\ (80\ \text{grams})}{30{,}000\ \text{grams}} = 1.6 \times 10^{-4}\ \text{day}^{-1}$$

Grit or soil ingestion rates are often expressed as a percent of total food intake per day. The rate therefore has units of g soil g^{-1} predator day^{-1}. The rate constant must be adjusted by multiplying by the predator biomass and dividing by the soil mass. Using a 10% soil ingestion factor and a total food intake rate of 0.1 g g^{-1} day, the rate k_6 would be

$$k_6 = \frac{0.1\ (0.1\ \text{g g}^{-1}\ \text{day}\ (80\ \text{grams})}{3.4 \times 10^8\ \text{grams}} = 2.3 \times 10^{-9}\ \text{day}^{-1}.$$

10.5.2.3 Clearance Rates--

Clearance rates are most often determined through feeding studies on particular species with specific chemicals and may be difficult to obtain. The available guidance for estimating these rates (which have units of day^{-1}) is given in Section 6 (specifically Table 6-42). For soil dwelling organisms, if the ingestion rate and bioconcentration factor (BCF) is known, then the expression

$$k_3 = \frac{k_2 \rho \Delta Z}{BCF \rho_o} \qquad (10\text{-}23)$$

in which

ΔZ is the representative soil depth (cm) and
ρ_o is the organism soil density (g cm^{-2})

10.5.3 Initial Pesticide Concentrations

For Model 1, the initial pesticide concentration in soil is easily estimated by taking the application rate (kg ha^{-1}) and dividing by the representative soil mass with the appropriate units conversions. Initial concentrations are input in μg g^{-1}. Therefore the concentration (C_s') may be found by

$$C_s' = \frac{10A}{\rho_s \Delta Z} \tag{10-24}$$

in which A is the application rate in kg ha^{-1}.

For Model 2 an equivalent daily loading rate (μg day^{-1}) to emulate multiple chemical applications is found by simply dividing the total application over the period by the length of the period in days.

10.5.4 Estimation of Parameters for Monte Carlo Analysis

The above techniques would be used to estimate mean values for Monte Carlo analysis. In addition, for each parameter, the coefficient of variation (CV), minimum and maximum and distribution type must be selected. If correlations between randomly generated parameters are desired, correlation coefficients must also be specified.

10.5.4.1 Coefficients of Variation (CV)--

The CV is a normalized measure of the spread of the uncertainty about the mean value of the parameter. It is equivalent to the standard deviation divided by the mean. Default CVs for each input parameter have been provided in the interactive and batch input sets. Table 10.2 shows their values.

Degradation and clearance rates--Specific guidance for degradation rates in soils is available. Rao and Davidson (1980) give CVs for soil degradation rates for approximately 30 herbicides, insecticides and fungicides. They ranged from 16.1% to 130.8%. A representative value is on the order of 50 to 100%. Specific guidance for CVs for clearance rates is largely unavailable to the authors. Calculated clearance rates for wood thrushes fed earthworms contaminated with dieldrin (Jeffries and Davis 1968) had a CV of 97% (n = 5). It is assumed that CVs for clearance rates would be similar, possibly higher than, the CVs for soil degradation.

Soil mass and animal biomass--CVs for biomasses can be obtained using ranges of counts or biomass density found in the literature. For instance, Lee (1985) gives a range of 0.5 to 20 g m^{-2} for earthworm populations in arable soils and Lofty (1974), a range of 2-40 g m^{-2}. Taking the range to 1 to 30 g m^{-2}, and assuming such a range represents approximately the 2.5%

and 97.5% quantile levels of a normal distribution (these values lie 2 standard deviations on either side of the mean, respectively), the mean is 15.5 g m^{-2}, and the CV is

$$CV = \frac{30 - 15.5}{2(15.5)} = .47 \text{ or } 47\%$$

The CV for the mass of the soil is determined by the uncertainty in the volume of soil (i.e., habitat area (A) and representative depth (d)) and the uncertainty in soil bulk density, ρ_s. Bulk densities for several soils have been estimated to have a CV of about 9% (Jury 1985). Selection of a representative depth is more uncertain, more so for less strongly adsorbed chemicals. Ideally, one could evaluate the aggregate uncertainty in the calculation of a representative depth by propagating the uncertainties in each of the parameters of the estimating equation. According to Jury (1985) estimates of the CV of solute velocity range from 36 to 194%. Therefore, a similar level of uncertainty would be associated with the depth of pesticide penetration. The authors are not knowledgeable about the CV of the estimate of habitat or territory. Assuming a 50% variability to size of territory, an upper bound for the CV soil mass could be found by (Taylor 1982)

$$CV = \frac{\delta M}{|M|} = \frac{\delta A}{|A|} + \frac{\delta d}{|d|} + \frac{\delta \rho_s}{|\rho_s|} \text{ or } \frac{\delta M}{|M|} = 0.5 + 1.94 + 0.09 = 2.53$$

or ~ 250%, In the case where the quantities A, d and ρ_s are independent (one would expect them to be in this case), a more reasonable estimate of the aggregate uncertainty is

$$\frac{\delta M}{|M|} = \sqrt{\left(\frac{\delta A}{A}\right)^2 + \left(\frac{\delta d}{d}\right)^2 + \left(\frac{\delta \rho}{\rho}\right)^2} = \sqrt{(0.5)^2 + (1.94)^2 + (0.09)^2}$$

$$= 2.01 \text{ or } \sim 200\%.$$

Ingestion (transfer) rates--CVs of ingestion rates can most likely be estimated with information given on the observed ranges for the species of interest. For instance, Lofty (1974) gives a range of 0.1 to 0.3 g g^{-1} day^{-1} for ingestion of soil by earthworms. Assuming that these numbers represent the 2.5 and 97.5 percentiles, the CV would be 25%.

Initial pesticide concentrations--The uncertainty in initial soil pesticide concentrations (Model 1) stems from uncertainty in the quotient of the application rate and the mass of affected soil. In a quotient, these uncertainties would sum to give an upper bound. To obtain an aggregate uncertainty, assuming independence of the quantities in the quotient, the root mean square of the fractional uncertainties of these quantities is calculated. The uncertainty in application rate is a function of the type of application equipment and meteorological conditions occurring during the spray event. Smith (1988, personal communication) reports that the CVs for granular application range from 40 to 70% and are approximately 25% for spray applications from ground equipment. Jury (1985) documents CVs of 60 to 130% for measured pesticide concentrations in soils. These CVs do not take into account the high variability associated with determining depth of pesticide penetration, however, and its impact on estimated concentrations.

10.5.4.2 Minimum and Maximum Values--

Minimum values for all the parameters should be zero or close to zero. Minimum values for masses (soil, mass biomass) should be set to values slightly greater than zero to avoid zero divides in the solutions to the model equations. Default maximum values in the batch and interactive data sets are 100 times the mean. This should be sufficient to insure that no truncation occurs on the upper end of distributions. It should be noted that normal distributions specified with low means and large CVs will result in frequent truncation of the distribution by rejection of negative values. If this happens, it is probably best to specify a log normal distribution type for the parameter.

10.5.4.3 Distribution Type--

Unless the user has specific knowledge about distribution type, the recommendation is to use the normal distribution. It should be pointed out that, when specifying a log normal distribution, the user inputs the arithmetic mean and CV into the program. The code internally calculates the mean and variance of the corresponding log normal distribution according to relationships in Yevjevich (1972).

10.5.4.4 Correlation Coefficients--

It is difficult to give meaningful quantitative guidelines for estimating correlation coefficients for these parameters. There is reason to suspect that soil degradation rates and clearances rates would be highly positively correlated. There may be weak positive correlations between the biomass of predator and prey (due to prey availability considerations). There is probably some correlation between ingestion rates of soil dwelling organisms and ingestion of soil. There is no reason to believe that soil mass or animal biomass is correlated with degradation or clearance rates. It is suggested that the user adopt either of three values:

- Zero for no correlation
- (±) 0.5 for weak correlation and
- (±) 0.9 for strong correlation

for use in simulations. It is also suggested that a simulation be made assuming independence of all parameters to test the importance of the correlations selected.

In order for the correlation matrix to be decomposed, it must be positive definite. While this has a precise mathematical reasoning, to the user it suggests that the correlation matrix "makes sense". For instance, if A is strongly positively correlated with B (i.e., when A is large, B is large) and A is strongly negatively correlated with C (i.e., when A is large C is small) then B must also be negatively correlated with C. If such rules are not followed, the user may find that the program terminates with a message to the output file indicating that the correlation matrix could not be decomposed.

10.6 OUTPUT FILES

Five output file are created when the model is run, SOIL.OUT, TLEVL1.OUT, TLEVL2.OUT, MCARLO.OUT, and the user specified output file. All of these files except the user specified output file are formatted for easy importation into LOTUS or a similar program. The results are stored in columns. If titles are printed at the top of a column they are bracketed by quotation marks (").

MCARLO.OUT contains all of the values of the variables that were generated by the random number generators. Figure 10.7 is an example of this file for a case of ten Monte Carlo simulations with nine randomly generated parameters. The first column in the file is the simulation number. If the run was deterministic this file will be empty.

TLEVL1.OUT and TLEVL2.OUT contain the calculated whole body concentrations and dosages from the model for the lower trophic level animal and higher trophic level animal respectively for each output period of the simulation. The files contain both the mean concentration for each

```
          INPUT PARAMETERS TO MODEL FOR EACH RUN OF THE MODEL

"RUN NO."  "DECAY1  "  "RATE12  "  "DECAY2  "  "RATE23  "  "DECAY3  "  "RATE13  "  "MASS1  "  "MASS2  "  "MASS3  "
   1   0.71619E-02 0.11450E-04 0.36964E-01 0.10261E-03  2.2893   0.14119E-08 0.60934E+09  29607.   74.718
   2   0.39054E-01 0.67061E-05 0.34664E-01 0.87746E-04  1.1236   0.25255E-09 0.61654E+09  35372.   78.674
   3   0.33652E-01 0.34689E-05 0.16503E-01 0.13347E-03 0.23010   0.64078E-09 0.50982E+09  38750.   89.670
   4   0.14461E-01 0.14915E-05 0.97345E-02 0.71499E-04  1.2630   0.10897E-08 0.61227E+09  35320.   88.249
   5   0.33230E-01 0.89781E-05 0.32909E-01 0.63236E-04 0.89912   0.70177E-09 0.59242E+09  38727.   83.542
   6   0.21745E-01 0.25538E-05 0.10526E-01 0.89265E-04 0.85588   0.84449E-09 0.57411E+09  45998.   94.120
   7   0.74350E-02 0.67093E-05 0.89383E-02 0.10901E-03 0.43908   0.45403E-09 0.60892E+09  33403.   80.538
   8   0.38008E-01 0.52353E-05 0.34344E-01 0.10172E-03  2.0887   0.29731E-09 0.56568E+09  30966.   84.132
   9   0.10473E-01 0.79452E-05 0.53647E-01 0.10186E-03  1.8503   0.15878E-08 0.55969E+09  45671.   66.551
  10   0.47201E-01 0.66163E-05 0.19863E-01 0.17247E-03  1.1216   0.24366E-09 0.60711E+09  37683.   79.414
```

Figure 10.7. Example of MCARLO.OUT output file.

period and the maximum concentration for the simulation. Figure 10.8 is an example of file TLEVL1.OUT. File TLEVL2.OUT is identical in format. The first line in the file contains two values, the total length of the simulation in days and the number of output periods. The first column in the file is the number of days during the simulation that the mean daily concentration exceeded THRESHO (the toxicity threshold in soil-dwelling organisms) or THRESHB (the toxicity threshold in the predator). The next 2*NCAT columns contain the mean whole body concentrations and dosages for each output period of the simulation. The values are ordered by concentration then dosage for each output period--i.e., concentration for period 1, dosage for period 1; concentration for period 2, dosage for period 2, etc.... The last column is the maximum concentration over the simulation period. If the simulation is run in deterministic mode file TLEVL2.OUT will be empty. File TLEVL1.OUT will contain the time series results of the simulation. The file will contain four columns of numbers as shown in Figure 10.9; the time (days), the soil concentration, the whole body concentration for the lower trophic level animal, and, the whole body concentration for the higher trophic level animal.

The final output file is the user specified output file. This file contains an echo of the input data and the results of the simulations. Statistics for both the lower and upper trophic levels are presented along with printer plots. The statistics and the plots correspond to the data found in files TLEVL1.OUT and TLEVL2.OUT. The file contains two type of printer plots as shown in Figures 10.10 and 10.11, one a histogram of the results and the other a CDF of the results. Results are presented for the number of days the concentration exceeded THRESHO and THRESHB, the mean concentration and the dosage for each trophic level and each output period, and, the maximum calculated concentration over the entire simulation period.

```
        365           3
"DAY" "CONC"       "DOSE"      "CONC"      "DOSE"      "CONC"      "DOSE"
   0   14.27        76.01       8.731       32.66      3.658        13.46
   0   7.304        31.65      0.4796      0.2917      0.9876E-02  0.2388E-02  17.25
   0   8.666        22.27       2.406      0.3928      0.3338      0.6250E-02  12.69
   0   13.32        30.81       11.19       5.480       4.605      0.9222      11.58
   0   7.534        31.70      0.7188      0.5878      0.2255E-01  0.9839E-02  16.63
   0   10.09        22.41       6.163       1.656       1.920      0.1139      12.13
 212   20.66        50.85       25.59       21.14       16.07       8.425      12.34
   0   7.393        31.87      0.5179      0.3331      0.1144E-01  0.3102E-02  28.74
   0   4.918        34.80       1.864       10.02      0.5166       2.750      12.68
                                                                              6.414
```

Figure 10.8. Example of TLEVL1.OUT output file when model is run in Monte Carlo mode.

10.7 EXAMPLE PROBLEM

This section presents an example problem to enable the user to benchmark a simulation on his own machine. The example problem is a Monte Carlo simulation run with the default parameters on either the batch input file or the interactive input sequence. A portion of the example output is given in Appendix A. The first portion of the example output is an echo of the inputs. Selected tabular outputs are also included. The first output shows, for the soil dwelling organisms, the statistics for number of days that the whole body concentration exceeded the threshold concentration set by the user. The statistics shown are the mean, standard deviation, CV,

```
"DAYS"        "SOIL"         "LOWER TROPHIC""UPPER TROPHIC"
""            "CONC"            "LEVEL"          "LEVEL"
    1        7.3514408       0.73944130       0.34082055E-01
    2        7.2058242        1.4495200       0.63996961E-01
    3        7.0630920        2.1311105       0.91883599E-01
    4        6.9231870        2.7850643       0.11839441
    5        6.7860533        3.4122099       0.14373889
    6        6.6516359        4.0133542       0.16799640
    7        6.5198810        4.5892825       0.19122636
    8        6.3907359        5.1407590       0.21347759
    9        6.2641488        5.6685278       0.23474922
   10        6.1400692        6.1733128       0.25510813
   11        6.0184474        6.6558186       0.27457043
   12        5.8992346        7.1167309       0.29314689
   13        5.7823832        7.5567171       0.31087541
   14        5.6678464        7.9764263       0.32780205
   15        5.5555783        8.3764903       0.34392114
   16        5.4455340        8.7575238       0.35926837
   17        5.3376694        9.1201247       0.37387263
   18        5.2319414        9.4648748       0.38776696
   19        5.1283077        9.7923400       0.40094832
   20        5.0267267        10.103071       0.41345403
   21        4.9271578        10.397602       0.42530490
   22        4.8295612        10.676456       0.43654408
   23        4.7338978        10.940137       0.44714213
   24        4.6401292        11.189140       0.45715069
   25        4.5482180        11.423942       0.46660754
   26        4.4581274        11.645009       0.47547985
   27        4.3698213        11.852795       0.48383697
   28        4.2832643        12.047739       0.49165982
   29        4.1984219        12.230269       0.49899449
   30        4.1152600        12.400803       0.50583809
   31        4.0337454        12.559743       0.51221586
```

Figure 10.9. Example of TLEVL.OUT output file when model is run in deterministic mode.

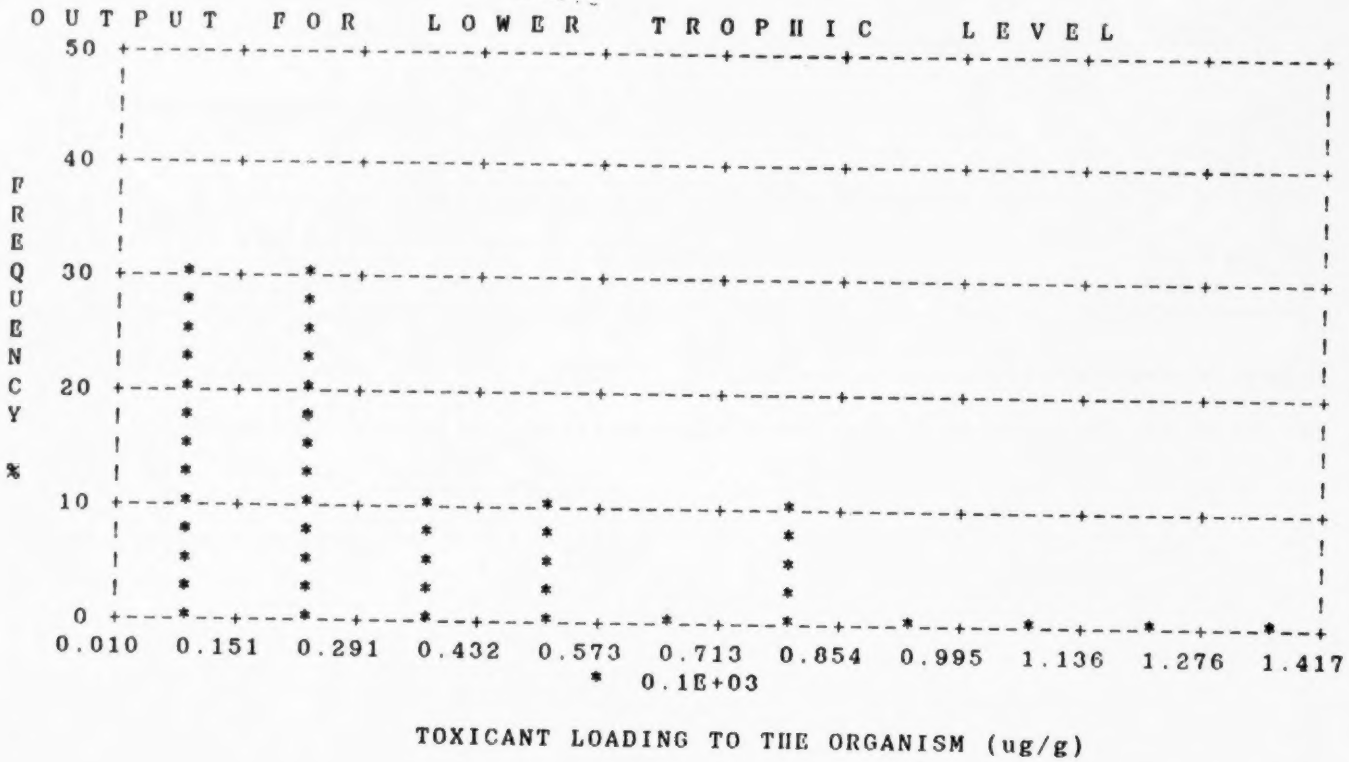


Figure 10.10. Example of histogram printer plot found in user specified output file.

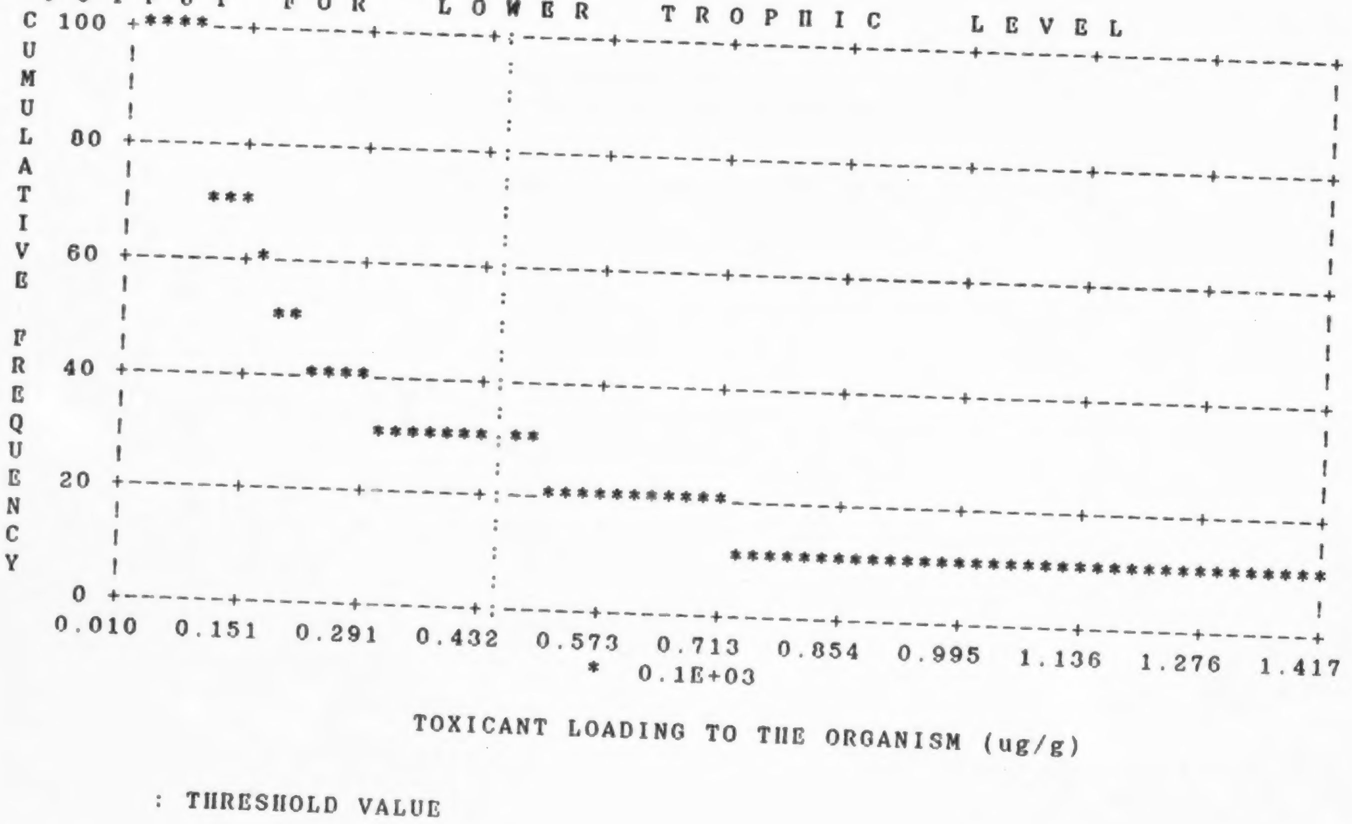


Figure 10.11. Example of CDF printer plot found in user specified output file.

maximum and minimum values. Due to differences in computational precision of various machines, it is likely that the output generated by the user may be slightly different. The statistics should be very similar however.

The next output is the tabular summary of statistics for the whole body concentration in the lower (soil dwelling) organism, for the first (90-day) output summary period. The next tabular output is summary statistics for dosage to the lower level organism (from the soil) during the first 90-day period. The next output is concentration statistics for the second 91-day period, followed by dosage statistics for that period. This is followed by concentration and dosage statistical summaries for the final 184-day period. The final tabular output for the lower trophic level is for the peak daily concentration during the entire simulation period.

The same tabular summaries are then presented for the higher trophic level. In the actual model output, relative frequency and cumulative relative frequency histograms are plotted for following each tabular summary.

SECTION 11

REFERENCES

Akesson, N.B., and W.E. Yates. 1976. Physical Parameters Relating to Pesticide Application. In: Pesticide Spray Application, Bebavior and Assessment: Workship Proceedings, Emeryville, CA, 1-2 March 1973. U.S. Pacific Southwest Forest and Range Experiment Station, Berkeley, CA. U.S. Dept. Agric. Forest Service. Gen. Tech Rep. PSW-15/1976.

Ambrose, R.B., S.I. Hill, and L.A. Mulkey. 1983. User's Manual for the Chemical Fate and Transport Model. TOXIWASP, Version I. EPA-600-3/83-005.

Ashton, F.M., and A.G. Crafts. 1981. Mode of Action of Herbicides, 2nd Ed. New York: John Wiley and Sons.

Bache, D.H., and S. Uk. 1975. Transport of Aerial Spray, II: Transport Within a Crop Canopy. Agricultural Meteorology 15:371-377.

Baker, P.B, E.R Hoebeke, J. Barnard, and T.D. Spittler. 1986. Arthropods Associated with Pesticide Leach Lines in Selected Orchards in Central New York. Env. Toxicol. and Chem. 5(1): 61-68.

Barker, R.J. 1958. Some notes on ecological effects of DDT sprayed elms. J. Wildlife Mgmt. 22:269-274.

Baver, L.D., W.H. Gardner, and W.R. Gardner. 1972. Soil Physics. Fourth ed. John Wiley & Sons, Inc., New York.

Beard, K.V., and H.R. Pruppacher. 1971. A Wind Tunnel Investigation of the Rate of Evaporation of Small Water Drops Falling at Terminal Velocity in Air. Journal of Atmospheric Science 28:1455-1464.

Bent, A.C. 1949. Life Histories of North American Thrushes, Kinglets, and Their Allies. Smithsonian Institute, U.S. National Museum, 196 p.

Biederbeck, V.O., C.A. Campbell, and A.E. Smith. 1987. Effects of Long Term 2,4-D Applications on Soil Biochemical Processes. Journal of Environmental Quality 16(3):257-262.

Boersma, L., F.T. Lindstrom, C. McFarlane, and E.L. McCoy. Uptake of Organic Chemicals by Plants: A Theoretical Model. In press.

Brakensiek, D.L., and Rawls, W.J. 1985. Prediction of Soil Water Properties for Hydrologic Modeling. In: Proceedings of Symposium Sponsored by Committee on Watershed Management, ASCE, Denver, Colorado.

Brackensiek, D.L., and W.J. Rawls. 1983. Green-Ampt Infiltration Model Parameters for Hydrologic Classification of Soils. In: Proceedings of Special Conference on Advances in Irrigation and Drainage, ASCE, Jackson, Wyoming.

Brady, N.C. 1974. The Nature and Properties of Soils. 8th. ed. New York: MacMillan Publishing Co.

Briggs, G.G., R.H. Bromilow, A.A. Evans, and M. Williams. 1983. Relationships between Lipophilicity and the Distribution of Non-ionized Chemicals in Barley Shoots following Uptake by Roots. Pesticide Science 14:492-500.

Briggs, G.G., R.H. Bromilow, and A.A. Evans. 1982. Relationship between Lipophilicity and Root Uptake and Translocation of Non-ionized Chemicals by Barley. Pesticide Science 13:495-504.

Burns, L.A., D.M. Cline, and R.R. Lassiter. 1982. Exposure Analysis Modeling System (EXAMS): User Manual and System Documentation. U.S. Environmental Protection Agency, Athens, Georgia. EPA-600/3-82-023. July.

Carsel, R.F., and R.S. Parrish. 1988. Developing Joint Probability Distributions of Soil Water Retention Characteristics. Water Resources Research 24(5):755-769.

Carsel, R.F., R.S. Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. Characterizing the Uncertainty of Pesticide Leaching in Agricultural soils. J. of Contam. Hydrol. 25: 111-124.

Carsel, R.F., C.N. Smith, L.A. Mulkey, J.D. Dean, and P. Jowise. 1984. User's Manual for the Pesticide Root Zone Model (PRZM): Release 1. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, Georgia. EPA-600/3-84-109.

Chapman, R.A., and P.C. Chapman. 1986. Persistence of Granular and EC Formulations of Chlorpyrifos in a Mineral and in Organic Soil Incubated in Open and Closed Containers. J. Environ. Sci. Health B21(6): 447-456.

Collett, N., and D.L. Harrison. 1968. Some Observations on the Effects of Using Organochlorine Sprays in an Orchard. N.Z.J. Sci. 11: 371-379.

Criddle, W.D. 1958. Methods of Computing Consumptive Use of Water. Proc. ASCE 84(IR1).

Dean, J.D., A.S. Donigian, Jr., and J.E. Rafferty. 1984. Development of a Mathematical Model to Evaluate Pesticide Exposure to Birds in Agricultural Ecosystems. Draft Report of Work Assignment No. 11, Contract No. 68-03-3116. U.S. Environmental Protection Agency, Athens, Georgia.

Dean, J.D. 1979. Determination of Irrigation Water Demand in Humid Climates. Master's Thesis, University of Georgia, Agricultural Engineering Department.

Dejonckheere, W., W. Steurbaut, O. Melkebeke, and R.H. Kips. 1983. Leaching of Aldicarb and Thiofanox, and Their Uptake in Soils by Sugarbeet Plants. Pesticide Sci. 14:99-107.

DeWeese, L.R., L.C. McEwan, G.L. Hensler, and B.E. Petersen. 1986. Organochlorine Contaminants in Passeriformes and Other Prey of the Peregrine Falcon in the Western United States. J. Env. Tox. and Chem. 5(7):675-694.

Donigian, A.S., Jr., C.S. Raju, and R.F. Carsel. 1986. Impact of Conservation Tillage on Environmental Pesticide Concentrations in Three Agricultural Regions. Prepared for U.S. EPA, Integrated Environmental Management Division, Office of Policy Analysis, Washington, D.C.

Donigian, A.S., Jr., and J.D. Dean. 1985. Nonpoint Source Models for Chemicals. In: Environmental Exposure from Chemicals, Vol. II. Boca Raton, Florida: LRC Press.

Dorst, J. 1974. The Life of Birds. Vol. 1. New York: Columbia Univ. Press.

Dumbauld, R.K., J.R. Bjorklund, and S.F. Saterlie. 1980. Computer Models for Predicting Aircraft Spray Dispersion and Deposition above and within Forest Canopies: User's Manual for the FSCBG Computer Program. Report No. 80-11. U.S.D.A. Forest Service, FPM-MAG, Davis, California.

Dumbauld, R.D., C.R. Bowman, and J.R. Rafferty. 1980. Optimum Swath Widths and Application Rates for Selected Aircraft and Meteorological Regimes. USDA Forest Service, Davis, CA. Rep No. TR-80-319-01.

Dumbauld, R.D., J.E. Rafferty, and J.R. Bjorklund, 1977. Prediction of Spray Behavior above and within a Forest Canopy. USDA Forest Service. Pacific N.W. Forest and Range Experiment Station, Portland, Oregon Rep. No. TR-77-308-01.

Dyer, A.J. 1974. A Review of Flux-Profile Relationships. Boundary-Layer Meteorology 7:363-372.

Dyer, A.J., and B.B. Hicks. 1970. Flux-Gradient Relationships in the Constant Flux Layer. Quarterly Journal of the Royal Meteorological Society 96:715-721.

Edwards, C.A. 1974. Macroarthropods. In: Biology of Plant Litter Decomposition, Vol 2, eds. C. H. Dickinson and G.J.F Pugh. New York: Academic Press.

El-Bayoumi, M.A., H.H. Shugart, Jr., and R.W. Wein. 1983/84. Modelling Succession of Eastern Canadian Mixedwood Forest. Ecol. Modelling 21:175-198.

Farner, D.S., J.R. King, and K.C. Parks. 1972. Avian Biology. New York: Academic Press.

Fletcher, J.S., M.J. Muhitch, D.R. Vann, J.C. McFarlane, and F.E. Benanati. 1985. PHYTOTOX Database Evaluation of Surrogate Plant Species Recommended by the U.S. Environmental Protection Agency and the Organization for Economic Cooperation and Development. Environ. TOX and Contam. 4(4): 523-532.

Freeze, R.A. 1975. Stochastic - Conceptual Analysis of One-Dimensional Groundwater Flow in Non-uniform Homogeneous Media. Water Res. Res. 11(5): 725-741.

Fuchs, N.A. 1959. Evaporation and Droplet Growth in Gaseous Media. New York: Pergamon Press.

Gibbs, G.H., J. Barnard, N.H. Peck, and M.T. Vittum. 1980. Soil and Air Temperature at Geneva, N.Y. Search Agriculture Number 5. New York State Agricultural Experimental Station, Cornell University, Ithaca, N.Y.

Green, W. Heber, and G.A. Ampt. 1911. Studies in Soil Physics. I. The Flow of Air and Water through Soils. J. Agri. Sci. 4:1-24.

Haan, C.T. 1977. Statistical Methods in Hydrology. Ames, Iowa: Iowa State University Press.

Haith, D.A., and R.C. Loehr, eds. 1979. Effectiveness of Soil and Water Conservation Practices for Pollution Control. U.S. Environmental Protection Agency, Athens, Georgia. EPA-600/3-79-106.

Harding, D.J.L., and R.A. Stuttard. 1974. Microarthropods. In: Biology of Plant Litter Decomposition, Vol. 2, eds. C.H. Dickinson and G.J.F. Pugh. New York: Academic Press.

Haque, A., and W. Ebing. Uptake, Accumulation, and Elimination of HCB and 2,4-D by the Terrestrial Slug, Deroceras reticulatum (Müller). Bull. Environ. Contam. Toxicol. 31, 727-733 (1983).

Hetrich, D.M., and L.M. McDowell-Boyer. 1984. User's Manual for TOXSCREEN: A Multimedia Screening-Level Program for Assessing the Potential Fate of Chemicals Released to the Environment. ORNL-6041, EPA-560/5-84-024.

Hill, E.F., R.G. Heath, J.W. Spann, and J.D. Williams. 1975. Lethal Dietary Toxicities of Environmental Pollutants to Birds. Special Sci. Rep. - Wildlife 191. U.S. Dept. of Interior, Fish and Wildlife Services Washington, D.C.

Jeffries and Davis. 1968. Dynamics of Dieldrin in Soil, Earthworms and Song Thrushes. J. Wildlife Management. 32: 441-456.

Johanson, R.C., J.C. Imhoff, and H.H. Davis, Jr. 1980. User's Manual for Hydrological Simulation Program--Fortran (HSPF). EPA-600/9-80-015.

Johnson, N.L., and S. Kotz. 1970. Distributions in Statistics: Continuous Univariate Distributions. Boston: Houghton Mifflin Company.

Jorde, D.G., G.L. Krapu, and R.O. Crawford. 1983. Feeding Ecology of Mallards Wintering in Nebraska. J. Wildlife Management 47(4): 1044-1053.

Jorgensen, S.E. 1984. Parameter Estimation in Toxic Substance Models. Ecol. Modeling 22:1-11.

Jury, W.A. 1985. Spatial Variability of Soil Physical Parameters in Solute Migration: A Critical Literature Review. Electric Power Research Institute Report No. EA-4228. Palo Alto, California.

Jury, W.A., W.F. Spencer and W.F. Farmer. 1984. Behavior Assessment Model for Trace Organics in Soil: III. Application of Screening Model. 13:573-579.

Jury, W.A., R. Grover, W.F. Spencer, and W.J. Farmer. 1983. Behavior Assessment Model for Trace Organics in Soil: I. Model Description. J. Environ. Qual., 12:558-564.

Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. Sorption of Hydrophobic Pollutants on Natural Sediments.

Kiekebusch, B.D., B.H. Edwards, J.N. Pavillin, and K.A. Coghlan-Jordan. 1981. Procedures for Predicting Transfers of Organic Substances in the Terrestrial Food Chain. Draft Report for Contract No. 68-03-3110. U.S. Environmental Protection Agency, Athens, Georgia.

Kirchner, T.B., and F.W. Whicker. 1984. Validation of PATHWAY. A Simulation Model of the Transport of Radionuclides through Agroecosystems. Ecological Modeling 22:21-44.

Lassey, K.R. 1982. The Interception and Retention of Aerosols by Vegetation - I. The Formulation of a Filtration Module. Atmospheric Environment 16(1):13-24.

Lee, K. E. 1985. Earthworms. Their Ecology and Relationships with Soils and Land Use. New York: Academic Press.

Linsley, R.K., Jr., M.A. Kohler, and J.L.H. Paulus. 1975. Hydrology for Engineers. New York: McGraw Hill

Lo, A.K. 1977. An Analytical-Empirical Method for Determining the Roughness Length and Zero-Plane Displacement. Boundary-Layer Meteorology 12:141-151.

Lofty, J. R. 1974. Oligochaetes. In: Biology of Plant Litter Decomposition, Vol. II, eds. C.H. Dickenson and G. J. F Pugh. New York: Academic Press.

Lyman, W.J., W.F. Reohl, and D.H. Rosenblatt. 1982. Handbook of Chemical Property Estimation Methods. New York: McGraw-Hill.

Matthews, G.A. 1979. Pesticide Application Methods. New York: Longman, Inc.

McDonald, J.E. 1960. An Aid to Computation of Terminal Fall Velocities of Spheres. Journal of Meteorology 17:463.

McFarlane, J.C., T. Pfleeger and John Fletcher. 1987. Transpiration Effect on the Uptake and Distribution of Bromacil, Nitrobenzene, and Phenol in Soybean Plants. J. Env. Qual. 16(4): 372-376.

McGrath et al., E.J. and D.C. Irving, 1973. Techniques for Efficient Monte Carlo Simulation, Volume II. Random Number Generation for Selected Probability Distributions. Report prepared for Office of Naval Research. Project No. NR 366-076/1-5-72, Code 462.

McKone, T.E., and D.W. Layton. 1986. Screening the Potential Risks of Toxic Substances Using a Multimedia Compartment Model. Lawrence Livermore National Laboratory Project No. UCRL-94548.

Mehlenbacher, L.A., and D.W.A. Whitfield. 1977. Modeling Thermal Eddy Diffusivity at Canopy Height. Boundary-Layer Meteorology 12:153-170.

Mejia J. M., and I. Rodriguez - Iturbe and J.R. Cordova. 1974. Multivariate Generation of Mixture of Normal and Log Normal Variables. Water Resources Research 10, (4):691-693.

Menzie, C.M. 1980. Metabolism of Pesticide Update III. U.S. Dept. of the Interior, Fish and Wildlife Service Spec. Sci. Rep. Wildlife No. 32. Washington D.C.

Mockus, V. 1972. Estimation of Direct Surface Runoff from Storm Rainfall. In: National Engineering Handbook. Section IV, Hydrology. U. S. Soil Conservation Report NEH-Notice 4-102. August.

Nash, R.G. 1980. Dissipation of Pesticides from soils. In: CREAMS: A Field Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems, W.G. Knisel, ed., U.S. Dept of Agriculture Conservation Res. Rep. No. 26. Washington, D.C.

Nash, R.G. 1974. Plant Uptakes of Insecticides, Fungicides and Fumigants from Soils. *In*: *Pesticides in Soil and Water*. Soil Sci. Soc. Am., Madison, Wisconsin.

Nielson, D.R., J.W. Biggar, and K.T. Erh. 1983. Spatial Variability of Field Measured Soil Water Properties. Hilgardia 42(7): 214-259.

Norstrom, R.J., T.P. Clark, D.A. Jeffrey, and H.T. Won. 1986. Dynamics of Organochlorine Compounds in Herring Gulls (Larus Argentatus): I. Distribution and Clearance of [^{14}C]DDE in Free-Living Herring Gulls (Larus Argentatus). Environmental and Toxicology and Chemistry, Vol. 5, pp. 41-48, 1986.

Odum, E.P. 1971. *Fundamentals of Ecology*. 3rd. ed. Philadelphia: W.B. Saunders Company.

Oliver, H.R. 1971. Wind Profiles in and above a Forest Canopy. Quarterly Journal of the Royal Meteorological Society 97:548-553.

Parmele, L.H., E.R. Lemon, and A.W. Taylor. 1972. Micrometeorological Measurement of Pesticide Vapor Flux from Bare Soil and Corn under Field Conditions. Water, Air, and Soil Pollution 1:433-451.

Patterson, M.R., T.J. Sworski, A.L. Sjoreen, M.G. Browman, C.C. Coutant, D.M. Hetrich, B.D. Murphy, and R.J. Raridon. 1984. A User's Manual for UTM-TOX, the Unified Transport Model. ORNL-6064.

Perkins, H.C. 1974. *Air Pollution*. New York: McGraw-Hill, Inc.

Picot, J.J.C. 1979. Comments on Droplet Spectrum Lower Limit and Droplet Evaporation. University of New Brunswick, Department of Chemical Engineering Report, Fredericton, New Brunswick, Canada.

Prandtl, L., and O.g. Tietjens. 1934. Fundamentals of Hydro- and Aeromecahnics. New York: Dover Publications, Inc.

Pruppacher, H.R., and R. Rasmussen. 1979. A Wind Tunnel Investigation of Evaporation of Large Water Drops Falling at Terminal Velocity in Air. Journal of Atmospheric Science 36:1255-1260.

Rafferty, J.E., and R.K. Dumbauld. 1980. Selection of Spray Operations Criteria for the Withlacoochee State Seed Orchard Project. USDA, Forest Service Methods Application Group Rep. No. 80-8. Davis, CA.

Rao, P.S.C., and R.J. Wagenet. 1985. Spatial Variability of Pesticides in Field Soils: Methods for Data Analysis and Consequences. Weed Sci. 33: 1-26.

Rao, P.S.C, and J.M. Davidson. 1980. Estimation of Pesticide Retention and Transformation Parameters Required in Nonpoint Source Pollution Models. *In*: Environmental Impact of Nonpoint Source Pollution, eds. M.R. Overcash and J.M Davidson. Ann Arbor, Michigan: Ann Arbor Sciences Publishers, Inc.

Rawls, W.J. 1983. Estimating Soil Bulk Density from Particle Size Analysis to Organic Matter Content. Soil Science, 135(2): 123-125.

Richards, L.A. 1931. Capillary Conduction of Liquids Through Porous Mediums. Physics 1:318-333.

Roberts, B.C., and H.W. Dorough. 1985. Hazards of Chemicals to Earthworms. Environmental Toxicology and Chemistry 4(3):307-323.

Rosenberg, N.J. 1974. Microclimate: The Biological Environment. New York: Wiley Interscience.

Ruppell, R.F., and C.W. Laughlin. 1976. Toxicity of some Pesticides to Earthworms. J. Kans. Entomol. Soc. So: 113-118.

Schnoor, J.L., C. Sato, D. McKechin and D. Sahoo. 1987. Processes, Coefficients, and Models for Simulating Toxic Organics and Heavy Metals in Surface Waters. WPA/600/3/3-87/015. U.S. EPA, Environmental Research Laboratory, Athens, Georgia.

Smith, A. 1932. Seasonal Subsoil Temperature Variations. J. Agr. Research 44:421-428.

Smith, C.N., and R.F. Carsel. 1984. Foliar Washoff of Pesticide (FWOP) Model: Development and Evaluation. Journal of Env. Sci. and Health.

Smith, R.L. 1966. Ecology and Field Biology. New York: Harper and Row Publishers. 2nd ed.

Soil Conservation Service, U.S. Department of Agriculture. 1972. SCS National Engineering Handbook, Section 4-Hydrology.

Spencer, W.F., W.A. Jury, and W.J. Farmer. 1984. Importance of Volatilization as a Pathway for Pesticide Loss from Forest Soils. In Chemical and Biological Controls In Forestry. American Chemistry Society, pp. 193-209.

Stanhill, G. 1969. A Simple Instrument for the Field Measurement of Turbulent Diffusion Flux. J. Applied Meteorology 8:504-513.

Stewart, B.A., D.A. Woolhiser, W.H. Wischmeier, J.H. Caro, and M.H. Fere. 1976. Control of Water Pollution from Cropland, Volume II: An Overview. U.S. Environmental Protection Agency, Athens, Georgia. EPA-600/2-75-026b.

Swanson, G.A., M.I. Meyer, and V.A. Adomaitis. 1985. Foods Consumed by Breeding Mallards on Wetlands of South Central North Dakota. J. Wildlife Management. 49(1):197-203.

Taylor, J. R. 1982. An Introduction to Error Analysis. Mill Valley, California: University Science Books.

Thibodeaux, L.J., and H.D. Scott. 1985. Air/Soil Exchange Coefficients. In: Environmental Exposure from Chemicals, Vol. I, eds. W.B. Neely and G.E. Blau, pp. 65-90, CRC Press, Inc.

Thibodeaux, L.J. 1979. Chemodynamics: Environmental Movement of Chemicals in Air, Water, and Soil. New York: John Wiley & Sons.

Thom, A.S., J.B. Stewart, H.R. Oliver, and J.H.C. Gash. 1975. Comparison of Aerodynamic and Energy Budget Estimates of Fluxes over a Pine Forest. Quarterly Journal of the Royal Meteorological Society 101:93-105.

Thompson, A.R, and C.A. Edwards. 1974. Effects of Pesticides on Nontarget Invertibrates in Freshwater and Soil. In: Pesticides in Soil and Water, W.D. Guenzis, ed. Soil. Sci. Soc. Am. Madison, Wisconsin.

Tinsley, I.J. 1979. Chemical Concepts in Pollutant Behavior. New York: John Wiley & Sons.

Todd, D.K. 1980. Groundwater Hydrology. Sec. Ed. NY: Wiley.

Todd, D.K. 1970. The Water Encyclopedia, Water Information Center, Port Washington, New York.

U.S. Department of Agriculture, Forest Service. 1984. Measurement of Drop Size Frequency from Nozzles used for Aerial Applications of Pesticides in Forests. October.

U.S. Department of Agriculture. 1980. CREAMS: A Field-Scale Model for Chemicals, Runoff and Erosion from Agricultural Management Systems, W.G. Knisel, ed., U.S. Dept. of Agriculture Conservation Res. Rep. No. 26. Washington, D.C.

Uk, S., and R.J. Courshee. 1982. Distribution and Likely Effectiveness of Spray Deposits Within a Cotton Canopy From Fine Ultralow-Volume Spray Applied by Aircraft. Pesticide Science 13:529-536.

van Genuchten, M. Th. 1978. Mass Transport in Saturated - Unsaturated Media: One Dimensional Solutions. Dept. of Civil Eng. Princeton University Res. Rep. 78-WR-11.

Van Gestel, C.A.M., and W. Ma. 1987. Toxicity and Bioaccumulation of Chlorinated Phenols in Earthworms. In: Vulnerability of Soil and Groundwater to Pollutants. Proceedings of the International Conference. March 30-April 3, 1987. Noordwijk on Zee, The Netherlands.

Wark, K., and C.F. Warner. 1976. Air Pollution: Its Origin and Control. New York: Harper & Row Publishers.

Welty, J.C. 1962. The Life of Birds. Philadelphia: W.B. Saunders Co.

Welty, J.C. 1975. The Life of Birds. Philadelphia: W.B. Saunders Co.

Willardson, L.S., and R.L. Hurst. 1965. Sample Size Estimates in Permeabilty Studies. ASCE J. of Irr. and Drainage. 91(IRI): 1-9.

Williams, J.R., C.A. Jones, and P.T. Dyke. 1988. The EPIC Model. U.S. Department of Agriculture. Ag. Res. Serv., Temple, Texas.

Williams, J.R., P.T. Dyke, W.W. Fuchs, V.W. Bensen, O.W. Rice, and E.D. Taylor. 1987. EPIC the Erosion-Productivity Impact Calculator. Volume II. User Manual. Draft document USDA, Agricultural Research Service, Economics Research Service, and Soil Conservation Service.

Williams, J.R., C.A. Jones, and P.T. Dyke. 1983. A Modeling Approach to Determining the Relationship between Erosion and Soil Productivity. Trans. ASAE 27:129-144.

Williams, J.R., C.A. Jones, and P.T. Dyke. 1983. EPIC - A Model for Assessing the Effects of Erosion on Soil Productivity. In: Analysis of Ecological Systems: State-of-the-Art in Ecological Modeling, eds. W.K. Lauenroth, G.V. Skogerboe, and M. Flug. New York: Elsevier Scientific Publishing Company.

Williams, J.R. 1975. Sediment Yield Prediction with Universe Equation Using Runoff Energy Factor. In: Present and Prospective Technology for Predicting Sediment Yields and Sources. U.S. Dept of Agric. ARS-S-40.

Wright, M.A. 1977. Effects of Benomyl and some other Systemic Fungicides on Earthworms. Ann. Appl. Biol. 87: 520-524.

Yevjevich, V. 1972. Probability and Statistics in Hydrology. Water Resources Publication, Littleton, Colorado.

APPENDIX A

ATEEAM EXAMPLE OUTPUT USING DEFAULT PARAMETER VALUES

```
          ****************************
          *                          *
          *                          *
          *         A - TEEAM        *
          *                          *
          *  ANALYTICAL TERRESTRIAL ECOSYSTEM
          *   EXPOSURE ASSESSMENT MODEL
          *                          *
          *       DECEMBER 1987      *
          *                          *
          ****************************


      Example simulation for documentation.Single application



                    I N P U T  D A T A


      NMCR      (NUMBER OF MONTE CARLO RUNS)        =   500

        NP      (NUMBER OF MODEL INPUT PARAMETERS
                 BEING VARIED)                      =     9


     NDAYS      (LENGTH OF SIMULATION PERIOD (DAYS) =   365

      NCAT      (NUMBER OF CATEGORIES TO DIVIDE
                 THE OUTPUT TIME SERIES INTO)       =     3
    IMODEL      Type of model used                        1


SIMULATION STARTED ON  1/ 1/1987
SIMULATION ENDED   ON 31/12/1987
```

```
        SUMMARY OF INPUT PARAMETERS

PAR NAME   INPUT MEAN    INPUT C.V.      DIST. MEAN.   DIST. STD      MINIMUM VALUE       MAXIMUM VALUE  DIST TYPE
DECAY1     0.2000E-01     1.000           0.2000E-01   0.2000E-01      0.0000E+00           10.00        NORMAL
RATE12     0.6700E-05    0.5000           0.6700E-05   0.3350E-05      0.0000E+00          0.1000E-02    NORMAL
DECAY2     0.2000E-01     1.000           0.2000E-01   0.2000E-01      0.0000E+00          0.1000        NORMAL
RATE23     0.1020E-03    0.5000           0.1020E-03   0.5100E-04      0.0000E+00          0.5000E-02    NORMAL
DECAY3      1.200         1.000            1.200        1.200          0.0000E+00           5.000        NORMAL
RATE13     0.7150E-09     1.000           0.7150E-09   0.7150E-09      0.0000E+00          0.1000E-04    NORMAL
MASS1      0.5630E+09    0.1000           0.5630E+09   0.5630E+08      0.1000              0.2700E+11    NORMAL
MASS2      0.3750E+05    0.1000           0.3750E+05    3750.          0.1000              0.3000E+07    NORMAL
MASS3       80.00        0.1000            80.00        8.000          0.1000               8000.        NORMAL
CONC1        7.500       0.0000E+00                                   0.0000E+00          10.00         CONSTANT
CONC2       0.0000E+00   0.0000E+00                                   0.0000E+00          1.000         CONSTANT
CONC3       0.0000E+00   0.0000E+00                                   0.0000E+00          1.000         CONSTANT
```

```
CORRELATION MATRIX

          DECAY1   RATE12   DECAY2   RATE23   DECAY3   RATE13   MASS1    MASS2    MASS3

DECAY1    1.0000   0 9500   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000

RATE12    0.9500   1.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000

DECAY2    0.0000   0.0000   1.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000

RATE23    0.0000   0.0000   0.0000   1.0000   0.0000   0.0000   0.0000   0.0000   0.0000

DECAY3    0.0000   0.0000   0.0000   0.0000   1.0000   0.0000   0.0000   0.0000   0.0000

RATE13    0.0000   0.0000   0.0000   0.0000   0.0000   1.0000   0.0000   0.0000   0.0000

MASS1     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   1.0000   0.0000   0.0000

MASS2     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   1.0000   0.0000

MASS3     0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   1.0000


     NSTRT      Seed used in random number generator          1234567

     543 MONTE CARLO RUNS REJECTED BECAUSE PARAMETER BOUNDS EXCEEDED
```

```
OUTPUT FOR LOWER TROPHIC LEVEL

NUMBER OF DAYS DURING SIMULATION PERIOD WHEN MEAN CONCENTRATION EXCEEDED  20.000    ug/g

                    Example simulation for documentation.Single application

                          N                       =  500
                          MEAN                    =  17.8
                          STANDARD DEVIATION      =  59.2
                          COEFFICIENT OF VARIATION =  3.33
                          MINIMUM VALUE           =  0.000E+00
                          MAXIMUM VALUE           =  345.
                          80th PERCENTILE         =  0.000E+00
                          85th PERCENTILE         =  0.000E+00
                          90th PERCENTILE         =  46.0
                          95th PERCENTILE         =  139.
                    ________________________________________________________
                     VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                   OR EXCEEDED
                    ________________________________________________________

                    0.000E+00      100.000
                                                      89.000
                     34.5           11.000
                                                       2.800
                     69.0            8.200
                                                       1.600
                     103.            6.600
                                                       1.400
                     138.            5.200
                                                       0.800
                     172.            4.400
                                                       0.800
                     207.            3.600
                                                       1.200
                     241.            2.400
                                                       0.400
                     276.            2.000
                                                       0.800
                     310.            1.200
                                                       1.000
                     345.            0.200
                    ________________________________________________________
```

```
OUTPUT FOR LOWER TROPHIC LEVEL

MEAN DAILY CONCENTRATION FROM     0 TO  120 DAYS


                      Example simulation for documentation.Single application

                          N                              =   500
                          MEAN                           =   10.2
                          STANDARD DEVIATION             =   4.91
                          COEFFICIENT OF VARIATION       =  0.480
                          MINIMUM VALUE                  =   2.71
                          MAXIMUM VALUE                  =   31.2
                          80th PERCENTILE                =   13.6
                          85th PERCENTILE                =   15.1
                          90th PERCENTILE                =   17.0
                          95th PERCENTILE                =   20.4
                      ------------------------------------------------------
                        VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                     OR EXCEEDED
                      ------------------------------------------------------

                        1.00         100.000
                                                         2.800
                        4.02          97.200
                                                        27.400
                        7.04          69.800
                                                        27.400
                        10.1          42.400
                                                        18.800
                        13.1          23.600
                                                        11.600
                        16.1          12.000
                                                         5.800
                        19.1           6.200
                                                         3.200
                        22.1           3.000
                                                         1.800
                        25.2           1.200
                                                         0.600
                        28.2           0.600
                                                         0.200
                        31.2           0.400
                      ------------------------------------------------------
```

```
OUTPUT FOR LOWER TROPHIC LEVEL

DOSAGE DURING THE PERIOD FROM     0 TO  120 DAYS


                    Example simulation for documentation.Single application

                          N                        =  500
                          MEAN                     =  33.8
                          STANDARD DEVIATION       =  10.3
                          COEFFICIENT OF VARIATION = 0.304
                          MINIMUM VALUE            =  15.7
                          MAXIMUM VALUE            =  79.6
                          80th PERCENTILE          =  41.4
                          85th PERCENTILE          =  44.4
                          90th PERCENTILE          =  49.2
                          95th PERCENTILE          =  54.0
                    ____________________________________________________
                     VALUE     % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                 OR EXCEEDED
                    ____________________________________________________

                     1.00        100.000
                                                     0.000
                     8.86        100.000
                                                     0.400
                     16.7         99.600
                                                    16.000
                     24.6         83.600
                                                    36.800
                     32.4         46.800
                                                    25.200
                     40.3         21.600
                                                    10.600
                     48.1         11.000
                                                     7.200
                     56.0          3.800
                                                     2.600
                     63.8          1.200
                                                     0.800
                     71.7          0.400
                                                     0.200
                     79.6          0.200
                    ____________________________________________________
```

```
OUTPUT FOR LOWER TROPHIC LEVEL

MEAN DAILY CONCENTRATION FROM   120 TO  243 DAYS

                         Example simulation for documentation.Single application

                              N                        =   500
                              MEAN                     =   5.62
                              STANDARD DEVIATION       =   6.83
                              COEFFICIENT OF VARIATION =   1.22
                              MINIMUM VALUE            =  0.127E-01
                              MAXIMUM VALUE            =   45.4
                              80th PERCENTILE          =   8.84
                              85th PERCENTILE          =   11.3
                              90th PERCENTILE          =   14.5
                              95th PERCENTILE          =   19.7
                         ______________________________________________
                          VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                        OR EXCEEDED
                         ______________________________________________

                         0.127E-01     100.000
                                                         59.600
                          4.55          40.400
                                                         20.800
                          9.08          19.600
                                                          8.200
                          13.6          11.400
                                                          5.200
                          18.2           6.200
                                                          2.000
                          22.7           4.200
                                                          2.200
                          27.2           2.000
                                                          1.200
                          31.8           0.800
                                                          0.200
                          36.3           0.600
                                                          0.200
                          40.8           0.400
                                                          0.200
                          45.4           0.200
                         ______________________________________________
```

```
O U T P U T   F O R   L O W E R   T R O P H I C   L E V E L


DOSAGE DURING THE PERIOD FROM   120 TO  243 DAYS


                     Example simulation for documentation.Single application

                             N                        =  500
                             MEAN                     =  6.44
                             STANDARD DEVIATION       =  10.4
                             COEFFICIENT OF VARIATION =  1.62
                             MINIMUM VALUE            = 0.165E-02
                             MAXIMUM VALUE            =  75.9
                             80th PERCENTILE          =  10.6
                             85th PERCENTILE          =  14.8
                             90th PERCENTILE          =  20.0
                             95th PERCENTILE          =  28.0
                     ----------------------------------------------------------
                      VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                   OR EXCEEDED
                     ----------------------------------------------------------

                     0.165E-02      100.000
                                                        74.800
                      7.60           25.200
                                                        10.600
                      15.2           14.600
                                                         6.400
                      22.8            8.200
                                                         4.000
                      30.4            4.200
                                                         1.400
                      38.0            2.800
                                                         1.800
                      45.6            1.000
                                                         0.600
                      53.2            0.400
                                                         0.200
                      60.8            0.200
                                                         0.000
                      68.4            0.200
                                                         0.000
                      75.9            0.200
                     ----------------------------------------------------------
```

```
OUTPUT FOR LOWER TROPHIC LEVEL

MEAN DAILY CONCENTRATION FROM  243 TO  365 DAYS

                    Example simulation for documentation.Single application

                           N                        =  500
                           MEAN                     =  2.84
                           STANDARD DEVIATION       =  5.64
                           COEFFICIENT OF VARIATION =  1.99
                           MINIMUM VALUE            = 0.101E-04
                           MAXIMUM VALUE            =  56.3
                           80th PERCENTILE          =  3.91
                           85th PERCENTILE          =  5.50
                           90th PERCENTILE          =  7.54
                           95th PERCENTILE          =  14.3
                    ___________________________________________________
                      VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                   OR EXCEEDED
                    ___________________________________________________

                    0.101E-04     100.000
                                                        85.400
                     5.63          14.600
                                                         7.200
                     11.3           7.400
                                                         4.000
                     16.9           3.400
                                                         2.200
                     22.5           1.200
                                                         0.400
                     28.2           0.800
                                                         0.200
                     33.8           0.600
                                                         0.200
                     39.4           0.400
                                                         0.200
                     45.0           0.200
                                                         0.000
                     50.7           0.200
                                                         0.200
                     56.3           0.000
                    ___________________________________________________
```

```
OUTPUT FOR LOWER TROPHIC LEVEL

DOSAGE DURING THE PERIOD FROM   243 TO  365 DAYS

                                    Example simulation for documentation.Single application

                                           N                         =  500
                                           MEAN                      =  2.95
                                           STANDARD DEVIATION        =  7.56
                                           COEFFICIENT OF VARIATION  =  2.56
                                           MINIMUM VALUE             =  0.107E-06
                                           MAXIMUM VALUE             =  70.1
                                           80th PERCENTILE           =  2.75
                                           85th PERCENTILE           =  5.07
                                           90th PERCENTILE           =  9.26
                                           95th PERCENTILE           =  16.3
                                    ______________________________________________________
                                     VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                                  OR EXCEEDED
                                    ______________________________________________________

                                    0.107E-06     100.000
                                                                      87.200
                                     7.01          12.800
                                                                       6.400
                                     14.0           6.400
                                                                       2.400
                                     21.0           4.000
                                                                       1.600
                                     28.0           2.400
                                                                       1.000
                                     35.1           1.400
                                                                       0.600
                                     42.1           0.800
                                                                       0.600
                                     49.1           0.200
                                                                       0.000
                                     56.1           0.200
                                                                       0.000
                                     63.1           0.200
                                                                       0.000
                                     70.1           0.200
                                    ______________________________________________________
```

OUTPUT FOR LOWER TROPHIC LEVEL

```
RESULTS FOR MAXIMUM CONCENTRATION


                     Example simulation for documentation.Single application

                            N                        =  500
                            MEAN                     =  14.0
                            STANDARD DEVIATION       =  6.17
                            COEFFICIENT OF VARIATION = 0.439
                            MINIMUM VALUE            =  4.49
                            MAXIMUM VALUE            =  61.8
                            80th PERCENTILE          =  17.5
                            85th PERCENTILE          =  19.0
                            90th PERCENTILE          =  21.1
                            95th PERCENTILE          =  25.6
                     ____________________________________________________
                      VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                    OR EXCEEDED
                     ____________________________________________________

                     1.00         100.000
                                                        5.000
                     7.08          95.000
                                                       48.600
                     13.2          46.400
                                                       31.800
                     19.2          14.600
                                                        9.200
                     25.3           5.400
                                                        3.200
                     31.4           2.200
                                                        1.400
                     37.5           0.800
                                                        0.400
                     43.6           0.400
                                                        0.200
                     49.6           0.200
                                                        0.000
                     55.7           0.200
                                                        0.200
                     61.8           0.000
                     ____________________________________________________
```

```
OUTPUT FOR  HIGHER  TROPHIC  LEVEL

     NUMBER OF DAYS DURING SIMULATION PERIOD WHEN MEAN CONCENTRATION EXCEEDED   4000.0     ug/g

                         Example simulation for documentation.Single application

                              N                          =   500
                              MEAN                       =  0.000E+00
                              STANDARD DEVIATION         =  0.000E+00
                              COEFFICIENT OF VARIATION = ??????????
                              MINIMUM VALUE              =  0.000E+00
                              MAXIMUM VALUE              =  0.000E+00
                              80th PERCENTILE            =  0.000E+00
                              85th PERCENTILE            =  0.000E+00
                              90th PERCENTILE            =  0.000E+00
                              95th PERCENTILE            =  0.000E+00
                         ________________________________________________
                           VALUE     % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                        OR EXCEEDED
                         ________________________________________________

                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                                                          0.000
                         0.000E+00      100.000
                         ________________________________________________
```

```
OUTPUT FOR HIGHER TROPHIC LEVEL

MEAN DAILY CONCENTRATION FROM    0 TO  120 DAYS

                          Example simulation for documentation.Single application

                                 N                        =   500
                                 MEAN                     =  0.930
                                 STANDARD DEVIATION       =   3.53
                                 COEFFICIENT OF VARIATION =   3.79
                                 MINIMUM VALUE            =  0.642E-02
                                 MAXIMUM VALUE            =   55.0
                                 80th PERCENTILE          =  0.753
                                 85th PERCENTILE          =   1.04
                                 90th PERCENTILE          =   1.57
                                 95th PERCENTILE          =   2.44
                          ___________________________________________________
                           VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                         OR EXCEEDED
                          ___________________________________________________

                          0.642E-02     100.000
                                                              98.400
                           5.50           1.600
                                                               0.400
                           11.0           1.200
                                                               0.200
                           16.5           1.000
                                                               0.400
                           22.0           0.600
                                                               0.200
                           27.5           0.400
                                                               0.000
                           33.0           0.400
                                                               0.000
                           38.5           0.400
                                                               0.200
                           44.0           0.200
                                                               0.000
                           49.5           0.200
                                                               0.000
                           55.0           0.200
                          ___________________________________________________
```

```
OUTPUT FOR HIGHER TROPHIC LEVEL

DOSAGE DURING THE PERIOD FROM     0 TO  120 DAYS


                              Example simulation for documentation.Single application

                                    N                        =   500
                                    MEAN                     =   60.9
                                    STANDARD DEVIATION       =   42.4
                                    COEFFICIENT OF VARIATION =  0.696
                                    MINIMUM VALUE            =  0.743E-01
                                    MAXIMUM VALUE            =   306.
                                    80th PERCENTILE          =   86.6
                                    85th PERCENTILE          =   101.
                                    90th PERCENTILE          =   116.
                                    95th PERCENTILE          =   147.
                              ________________________________________________________
                                VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                              OR EXCEEDED
                              ________________________________________________________

                              0.743E-01       100.000
                                                                  23.200
                               30.6            76.800
                                                                  37.800
                               61.2            39.000
                                                                  21.400
                               91.8            17.600
                                                                   8.600
                               122.             9.000
                                                                   5.000
                               153.             4.000
                                                                   2.200
                               184.             1.800
                                                                   1.000
                               214.             0.800
                                                                   0.400
                               245.             0.400
                                                                   0.200
                               275.             0.200
                                                                   0.000
                               306.             0.200
                              ________________________________________________________
```

```
OUTPUT FOR HIGHER TROPHIC LEVEL

MEAN DAILY CONCENTRATION FROM   120 TO  243 DAYS

                    Example simulation for documentation.Single application

                            N                        =   500
                            MEAN                     =  0.755
                            STANDARD DEVIATION       =   4.80
                            COEFFICIENT OF VARIATION =   6.36
                            MINIMUM VALUE            =  0.362E-03
                            MAXIMUM VALUE            =   84.4
                            80th PERCENTILE          =  0.414
                            85th PERCENTILE          =  0.605
                            90th PERCENTILE          =  0.862
                            95th PERCENTILE          =   1.89
                    ________________________________________________________
                     VALUE        % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                     OR EXCEEDED
                    ________________________________________________________

                    0.362E-03      100.000
                                                          99.000
                     8.44            1.000
                                                           0.200
                     16.9            0.800
                                                           0.200
                     25.3            0.600
                                                           0.000
                     33.8            0.600
                                                           0.200
                     42.2            0.400
                                                           0.200
                     50.6            0.200
                                                           0.000
                     59.1            0.200
                                                           0.000
                     67.5            0.200
                                                           0.000
                     76.0            0.200
                                                           0.200
                     84.4            0.000
                    ________________________________________________________
```

```
OUTPUT FOR HIGHER TROPHIC LEVEL

DOSAGE DURING THE PERIOD FROM   120 TO  243 DAYS

                    Example simulation for documentation.Single application

                        N                        =   500
                        MEAN                     =   34.6
                        STANDARD DEVIATION       =   50.0
                        COEFFICIENT OF VARIATION =   1.45
                        MINIMUM VALUE            =  0.666E-01
                        MAXIMUM VALUE            =   397.
                        80th PERCENTILE          =   53.1
                        85th PERCENTILE          =   64.2
                        90th PERCENTILE          =   81.9
                        95th PERCENTILE          =   142.
                    ____________________________________________________
                     VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                  OR EXCEEDED
                    ____________________________________________________

                    0.666E-01     100.000
                                                       72.400
                     39.8          27.600
                                                       16.800
                     79.5          10.800
                                                        4.200
                     119.           6.600
                                                        3.600
                     159.           3.000
                                                        1.000
                     199.           2.000
                                                        1.000
                     238.           1.000
                                                        0.200
                     278.           0.800
                                                        0.400
                     318.           0.400
                                                        0.200
                     358.           0.200
                                                        0.000
                     397.           0.200
                    ____________________________________________________
```

```
OUTPUT FOR HIGHER TROPHIC LEVEL

MEAN DAILY CONCENTRATION FROM  243 TO  365 DAYS

                              Example simulation for documentation.Single application

                                   N                        =  500
                                   MEAN                     = 0.372
                                   STANDARD DEVIATION       =  2.36
                                   COEFFICIENT OF VARIATION =  6.36
                                   MINIMUM VALUE            = 0.287E-06
                                   MAXIMUM VALUE            =  40.4
                                   80th PERCENTILE          = 0.167
                                   85th PERCENTILE          = 0.233
                                   90th PERCENTILE          = 0.428
                                   95th PERCENTILE          =  1.12
                              ________________________________________________________
                                VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                              OR EXCEEDED
                              ________________________________________________________

                              0.287E-06       100.000
                                                                  98.600
                                4.04            1.400
                                                                   0.600
                                8.08            0.800
                                                                   0.000
                                12.1            0.800
                                                                   0.400
                                16.2            0.400
                                                                   0.000
                                20.2            0.400
                                                                   0.000
                                24.2            0.400
                                                                   0.200
                                28.3            0.200
                                                                   0.000
                                32.3            0.200
                                                                   0.000
                                36.4            0.200
                                                                   0.000
                                40.4            0.200
                              ________________________________________________________
```

```
OUTPUT FOR HIGHER TROPHIC LEVEL

DOSAGE DURING THE PERIOD FROM  243 TO  365 DAYS


                    Example simulation for documentation.Single application

                           N                        =   500
                           MEAN                     =   17.4
                           STANDARD DEVIATION       =   40.5
                           COEFFICIENT OF VARIATION =   2.33
                           MINIMUM VALUE            =  0.645E-04
                           MAXIMUM VALUE            =   422.
                           80th PERCENTILE          =   22.3
                           85th PERCENTILE          =   30.2
                           90th PERCENTILE          =   41.6
                           95th PERCENTILE          =   86.6
                  ____________________________________________________
                   VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                 OR EXCEEDED
                  ____________________________________________________

                  0.645E-04     100.000
                                                      90.600
                   42.2           9.400
                                                       4.200
                   84.4           5.200
                                                       2.800
                   127.           2.400
                                                       0.600
                   169.           1.800
                                                       1.000
                   211.           0.800
                                                       0.200
                   253.           0.600
                                                       0.000
                   295.           0.600
                                                       0.400
                   338.           0.200
                                                       0.000
                   380.           0.200
                                                       0.000
                   422.           0.200
                  ____________________________________________________
```

```
OUTPUT FOR HIGHER TROPHIC LEVEL

RESULTS FOR MAXIMUM CONCENTRATION


                    Example simulation for documentation.Single application

                           N                        =  500
                           MEAN                     =  1.37
                           STANDARD DEVIATION       =  5.86
                           COEFFICIENT OF VARIATION =  4.28
                           MINIMUM VALUE            =  0.815E-02
                           MAXIMUM VALUE            =  97.7
                           80th PERCENTILE          =  1.06
                           85th PERCENTILE          =  1.39
                           90th PERCENTILE          =  2.11
                           95th PERCENTILE          =  3.48
                    ------------------------------------------------------
                    VALUE      % OF TIME EQUALLED  % OF TIME IN INTERVAL
                                 OR EXCEEDED
                    ------------------------------------------------------

                    0.815E-02     100.000
                                                      98.800
                     9.78           1.200
                                                       0.200
                     19.6           1.000
                                                       0.400
                     29.3           0.600
                                                       0.000
                     39.1           0.600
                                                       0.200
                     48.9           0.400
                                                       0.000
                     58.7           0.400
                                                       0.200
                     68.4           0.200
                                                       0.000
                     78.2           0.200
                                                       0.000
                     88.0           0.200
                                                       0.000
                     97.7           0.200
                    ------------------------------------------------------
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